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As Unit 1621 Prove Number 2 2049 Location (R. de Roune) 524 (Mailler 4) 271 Results Format Preferred (chele): PAPER DISE To easure as efficient and quality secreb, please much a copy of the cover them, clause, and obstract or fill out the following: Title of invention; Bord works ad Inventors (p. cose provide full union) _ 178 E18

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STRUCTURE FILE UPDATES: 11 MAY 2008 HIGHEST RN 1020256-26-1
DICTIONARY FILE UPDATES: 11 MAY 2008 HIGHEST RN 1020256-26-1
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=> file zcaplus
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

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=> d stat que L40
L22
            19 SEA FILE=ZCAPLUS ABB=ON PLU=ON BIT R?/AU
1.23
            89 SEA FILE=ZCAPLUS ABB=ON PLU=ON GIBLIN G?/AU
L24
          2354 SEA FILE-ZCAPLUS ABB-ON PLU-ON HALL A?/AU
L25
          319 SEA FILE=ZCAPLUS ABB=ON PLU=ON HURST D?/AU
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          1179 SEA FILE=ZCAPLUS ABB=ON PLU=ON MILLER N?/AU
L28
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            2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L27 AND L28
L35
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L36
           19 SEA FILE=ZCAPLUS ABB=ON PLU=ON L30 AND (L31 OR L32 OR L33 OR
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L37
L38
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=> file medline embase biosis wpix

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L25	319	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	HURST D?/AU	
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L28	13	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	SCOCCITTI T?/AU	
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		L27 OR L28)			
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		L28)			
L32	18	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L25 AND (L26 OR L27	7 OR L28)
L33	5	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L26 AND (L27 OR L28	3)
L34	2	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L27 AND L28	
L35	7	SEA FILE=ZCAPLUS #	ABB=ON PLU=ON	L29 AND (L30 OR L31	L OR L32 OR
		L33 OR L34)			
L36	19	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L30 AND (L31 OR L32	OR L33 OR
		L34)			
L37	17	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L31 AND (L32 OR L33	3 OR L34)
L38	4	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L32 AND (L33 OR L34	1)
L39	2	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	L33 AND L34	
L40	21	SEA FILE=ZCAPLUS A	ABB=ON PLU=ON	(L35 OR L36 OR L37	OR L38 OR
		L39)			
L43	27	SEA L40			

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L49 22 DUP REM L40 L43 (26 DUPLICATES REMOVED)
ANSWERS '1-21' FROM FILE ZCAPLUS
ANSWER '22' FROM FILE BIOSIS

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L49 ANSWER 1 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2008:70761 ZCAPLUS Full-text

DOCUMENT NUMBER: 148:168573

TITLE: Indole derivatives as EP1 ligands, their preparation, pharmaceutical compositions, and use in therapy

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Horst,
David Nigel; Scoccitti, Tiziana; Theobald, Pamela Joan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 47pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATEN	T NO.			KIN	D	DATE		i	APPL	ICAT	ION	NO.		D	ATE	
					-											
WO 20	080067	90		A1		2008	0117	1	vio 2	007-	EP56	936		2	0070	709
W	: AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,
	CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	FI,
	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,
	KM,	KN,	KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ME,
	MG,	MK,	MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,
	PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,
	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW				
R	W: AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
	IS,	IT,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,
	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,
	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,
	BY,	KG,	KZ,	MD,	RU,	TJ,	TM									
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OTHER SOUR	CE(S):			MAR	PAT	148:	1685	73								

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to indole derivs. of formula I, which are ligands for the prostanoid EP1 receptor. In compds. I, Rl is H, Me, CF3, Cl, F, or Br; R2 is Et, Pr, iso-Pr, iso-Bu, 2,2-dimethylpropyl, 3,3-dimethylbutyl.

(un) substituted benzyl, 2,2,2-trifluoroethyl, or isobutanoyl; R3 is substituted oxazolyl, substituted thiazolyl, substituted thiazolylmethyl, substituted pyridinyl, substituted furyl, substituted thienyl, or substituted phenyl; and X is CH or N. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I together with a pharmaceutical carrier and/or excipient, as well as to the use of the compns. for the treatment of conditions mediated by the action of prostaglandin E2 (PGE2) on the EP1 receptor, such as pain, inflammatory disorders, and neurodegenerative disorders. Acylation of 6-chloroindole with propanovl chloride followed by hydride reduction resulted in the formation of indole II, which underwent substitution of Et 2-bromo-4-thiazolecarboxylate and ester hydrolysis to give N-(thiazolyl)indole III. Several compds. of the invention, e.g., III, expressed pIC50 values above 7 for their affinity towards the prostanoid EP1 receptor and pKi values above 7.0 in a human EP1 calcium mobilization functional assay.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 2 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

2008:462767 ZCAPLUS Full-text ACCESSION NUMBER:

TITLE: Discovery of a novel indole series of EP1 receptor

antagonists by scaffold hopping

AUTHOR(S): Hall, Adrian; Billinton, Andy; Brown, Susan H.;

Chowdhury, Anita; Giblin, Gerard M. P.; Goldsmith, Paul; Hurst, David N.; Navlor, Alan; Patel, Sadhana;

Scoccitti, Tiziana; Theobald, Pamela J.

CORPORATE SOURCE: Neurology Centre of Excellence for Drug Discovery,

GlaxoSmithKline, Harlow, Essex, CM19 5AW, UK SOURCE:

Bioorganic & Medicinal Chemistry Letters (2008),

18(8), 2684-2690

CODEN: BMCLE8: ISSN: 0960-894X

Elsevier Ltd. PUBLISHER: DOCUMENT TYPE: Journal

LANGUAGE: English

AB We describe the medicinal chemical approach that generated a novel indole series of EP1 receptor antagonists. The SAR of this new template was evaluated and culminated in the identification of compound 12g which demonstrated in vivo efficacy in a preclin. model of inflammatory pain.

L49 ANSWER 3 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2008:324741 ZCAPLUS Full-text

TITLE: Novel methylene-linked heterocyclic EP1 receptor

antagonists

AUTHOR(S): Hall, Adrian; Bit, Rino A.; Brown, Susan H.;

Chowdhury, Anita; Giblin, Gerard M. P.; Burst, David N.; Kilford, Jan R.; Lewell, Xiao; Naylor,

Alan; Scoccitti, Tiziana

CORPORATE SOURCE: Neurology Centre of Excellence for Drug Discovery,

GlaxoSmithKline, New Frontiers Science Park, Harlow,

Essex, CM19 5AW, UK

Bioorganic & Medicinal Chemistry Letters (2008), SOURCE:

18(5), 1592-1597

CODEN: BMCLE8: ISSN: 0960-894X

PUBLISHER: Elsevier Ltd. DOCUMENT TYPE: Journal

LANGUAGE: English

We describe the SAR, in terms of heterocyclic replacements, for a series of pyrazole EP1 receptor antagonists. This study led to the identification of several aromatic heterocyclic replacements for the pyrazole in the original

compound Investigation of replacements for the methylene linker uncovered disparate SAR in the thiazole and pyridine series.

L49 ANSWER 4 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2007:1302250 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:541735

TITLE: Preparation of substituted 2-benzylpyridine compounds

for treating a condition mediated by the action of

PGE2 at EP1 receptors

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Hurst,

David Nigel; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 58pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATEN	IT N	ю.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D	ATE	
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WO 20	0071	2875	52		A1		2007	1115	1	WO 2	007-	EP54:	254		20	0070	502
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		CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,
		GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,
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		RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,	TR,	TT,
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F	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
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		ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,
		GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,
		BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM									
PRIORITY A	APPL	N. 1	INFO	. :						GB 2	006-	3825		1	A 20	0060	504
OTHER SOUP	RCE (S):			MAR	PAT	147:	5417	35								

GI

AB The title compds. I [R1 = halo; X = O or S; R2 = iso-Bu or (un)substituted CH2Ph; R3 = CONH(CH2)mR4, NHCO2R5, CH(OH)CF3, etc.; R4 = H, alkyl, cycloalkyl, Ph or pyridyl; R5 = tert-Bu; m = 0-11 which bind with high affinity to the EP1 receptor, were prepared E.g., a multi-step synthesis of II, starting from 4chlorophenol and benzyl bromide, was given. Exemplified compds. I were evaluated in various assays (data given). Pharmaceutical composition comprising compound I is disclosed.

REFERENCE COUNT: THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS 2 RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 5 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5 2007:79571 ZCAPLUS Full-text

ACCESSION NUMBER: DOCUMENT NUMBER: 146:220141

The discovery of 6-[2-(5-chloro-2-{[(2,4-TITLE:

> difluorophenyl)methyl]oxy}phenyl)-1-cyclopenten-1-yl]-2-pyridinecarboxylic acid, GW848687X, a potent and selective prostaglandin EP1 receptor antagonist for

the treatment of inflammatory pain AUTHOR(S):

Giblin, Gerard M. P.; Bit, Pino A.; Brown, Susan H.; Chaignot, Helene M.; Chowdhury, Anita; Chessell, Iain P.; Clayton, Nicholas M.; Coleman, Tanya; Hall, Adrian; Hammond, Beverley; Hurst, David N.; Michel, Anton D.; Navlor, Alan; Novelli, Riccardo; Scoccitti, Tiziana; Spalding, David; Tang, Sac P.; Wilson, Alex

W.; Wilson, Rich

CORPORATE SOURCE: Department of Medicinal Chemistry and DMPK, New Frontiers Science Park, Essex, CM19 5AW, UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007),

17(2), 385-389

CODEN: BMCLE8; ISSN: 0960-894X

Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

PUBLISHER:

AB

The discovery of a series of selective EP1 receptor antagonists based on a 1,2-diarylcyclopentene template is described. After defining the structural requirements for EP1 potency and selectivity, heterocyclic rings were incorporated to reduce log D and improve in vitro pharmacokinetic properties. The 2.6-substituted pyridines and pyridazines gave an appropriate balance of potency, in vivo pharmacokinetic properties and a low potential for inhibiting

a range of CYP450 enzymes. From this series, GW848687X (I) was shown to have an excellent profile in models of inflammatory pain and was selected as a development candidate.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 6 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 2006:1157169 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:471519

TITLE: Preparation of pyrazole compounds as EP1 prostaglandin

receptor antagonists INVENTOR(S): Conway, Elizabeth Ann; Giblio, Gerard Martin Paul;

Gibson, Mairi; Hall, Adrian; Hayhow, Thomas George Christopher; Healy, Mark Patrick; Hurst, David Nigel; Kilford, Ian Reginald; McKeown, Stephen Carl; Navlor, Alan; Price, Helen Susanne; Rawlings,

Derek Anthony

PATENT ASSIGNEE(S): Glaxo Group Limited, UK PCT Int. Appl., 203pp. SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2006114313	A1 20061102	WO 2006-EP3919	20060424
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,
CN, CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KM, KN, KP, KR,
KZ, LC, LK,	LR, LS, LT, LU,	LV, LY, MA, MD, MG,	MK, MN, MW, MX,
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VN, YU, ZA,	ZM, ZW		
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KG, KZ, MD,	RU, TJ, TM		
EP 1874303	A1 20080109	EP 2006-742719	20060424
R: AT, BE, BG,	CH, CY, CZ, DE,	DK, EE, ES, FI, FR,	GB, GR, HU, IE,
IS, IT, LI,	LT, LU, LV, MC,	NL, PL, PT, RO, SE,	SI, SK, TR, HR
PRIORITY APPLN. INFO.:		GB 2005-8472	A 20050426
		WO 2006-EP3919	W 20060424
OTHER SOURCE(S):	MARPAT 145:4715	19	

GI

AB Pyrazoles (shown as I; variables defined below; e.g. 1,1-dimethylethyl [1-[[5chloro-2-((phenylmethyl)oxylphenyl]methyl]-5-methyl-1H-pyrazol-3- yl]carbamate (1)) or a pharmaceutically acceptable derivative thereof, a process for the preparation of such compds., pharmaceutical compns. comprising such compds. and the use of such compds. in medicine are disclosed. Although the methods of preparation are not claimed, prepns. and/or characterization data for .apprx.500 examples of I are included. For example, 1 was prepared from 1-[[5-chloro-2-[(phenylmethyl)oxylphenyl]methyl]-5-methyl-1H-pyrazole-3carboxylic acid, Et3N, and Ph2P(O)N3 in tBuOH; the starting acid was prepared by saponification of the Et ester, which was prepared by O-benzylation of Et 1-[(5-chloro-2-hydroxyphenyl)methyl]-5-methyl-1H-pyrazole-3-carboxylate (preparation of similar compound described). For I: Z is O, S, SO or SO2; Rx is (un) substituted C2-10alkyl, C2-10alkenyl, C2-10alkynyl, CQaQb-heterocyclyl, CQaQb-bicyclic heterocyclyl, or CQaQb-aryl; R1 is CONR3R4, NR3CO2R5, NR3COR6, OCONR3R7, tetrazolyl, oxazolin-2-yl, oxazol-2-yl, benzoxazol-2-yl, pyrrolidinonyl, isoindoledionyl, dihydroisoindolonyl, or (un)substituted SO2NHCOaryl; or R1 is (un)substituted imidazolyl or 1,2,4-triazolyl wherein optionally the imidazole or 1,2,4-triazole ring is fused to give an (un) substituted bicyclic or tricyclic ring system; or R1 = 4-R9-2oxopiperazin-1-yl. R2a and R2b = H, halo, CN, SO2alkyl, SR3, NO2, or (un) substituted alkyl or alkoxy; R3 is H or C1-4alkyl; R4 is H, OH, (un) substituted alkyl, aryl, heterocyclyl, bicyclic heterocyclyl, COcOdaryl, CQcQdheterocyclyl, or CQcQdbicyclic heterocyclyl, or SO2R8; R5 is (un) substituted C1-4alkyl, substituted cyclohexyl, Ph. et al.; R6 is alkyl or (un) substituted aryl, heterocyclyl, bicyclic heterocyclyl, CQcQd-Y-aryl, CQcQd-Y-heterocyclyl or CQcQd-Y-bicyclic heterocyclyl; R7 is (un)substituted alkyl, alkenyl, aryl, or CQcQdaryl; R8 is (un)substituted alkyl, aryl or heterocyclyl. R9 is (un)substituted alkyl, alkenyl, (un)substituted CQcQd-Yarvl, (un)substituted COcOd-Y-heterocyclyl or (un)substituted COcOd-Y-bicyclic heterocyclyl; R10 and R11 = H, F and alkyl; or R10 and R11 together with the C to which they are attached form a cycloalkyl ring, optionally containing up to one heteroatom = O, S, NH or N-alkyl; and Y is CH2 or a bond; Qa and Qb = H, CH3 and F; Qc and Qd = H, CH3 and F; addnl. details including provisos are given in the claims. Results are summarized for a binding assay for the human prostanoid EP1 receptor, a human EP1 Ca mobilization assay and for a human EP3 Ca mobilization assay for many examples of I.

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 7 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7

2006:1147656 ZCAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 145:471518 TITLE:

Preparation of oxazole and thiazole compounds as EP1

prostaglandin receptor antagonists

Bit, Pino Antonio; Hall, Adrian; Hurst, David

Nicel: Scoccitti, Tiziana

Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 124pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent.

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

INVENTOR(S):

PAT	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE	
						-									-		
WO	2006	1142	74		A1		2006	1102		WO 2	006-	EP38	10		2	0060	424
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
            MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN. YU. ZA. ZM. ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     EP 1874776
                         A1
                               20080109
                                          EP 2006-742682
                                                                  20060424
         R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR
                                                            A 20050426
PRIORITY APPLN. INFO.:
                                           GB 2005-8463
                                            WO 2006-EP3810
                                                              W 20060424
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OTHER SOURCE(S): GT

MARPAT 145:471518

AB Oxazoles and thiazoles (shown as I; variables defined below; e.g. 2-[[5chloro-2-[(phenylmethyl)oxylphenyl]methyl]-1.3-thiazole-4-carboxylic acid (1)) or a pharmaceutically acceptable derivative thereof, a process for the preparation of such compds., pharmaceutical compns. comprising such compds. and the use of such compds. in medicine are disclosed. Although the methods of preparation are not claimed, prepns. and/or characterization data for .apprx.180 examples of I are included. For example, 1 was prepared by saponification of the Et ester, which was prepared by cyclization of Et bromopyruvate with 2-[5-chloro-2-[(phenylmethyl)oxylphenyl]ethanethioamide . which was prepared from Lawesson's Reagent and 2-[5-chloro-2-[(phenylmethyl)oxy]phenyl]acetamide, which was prepared from [5-chloro-2-[(phenylmethyl)oxy]phenyl]acetic acid, which was prepared from the Et ester, which was prepared from 1-[5-chloro-2- [(phenylmethyl)oxy]phenyl]ethanone, which was prepared from benzyl bromide and 1-(5-chloro-2hydroxyphenyl)ethanone. Results are summarized for a binding assay for the human prostanoid EP1 receptor, a human EP1 Ca mobilization assay and for a human EP3 Ca mobilization assay for many examples of I. For I: either Y' is CH and Y'' is O or S, or Y' is O or S and Y is CH thus forming an exazole or a thiazole ring; X is CR7R8, O, NR4, S, SO, or SO2, or X is a bond; Z is O, S, SO or SO2; Rx is (un) substituted C3-10alkyl, C3-10alkenyl, C3-10alkynyl, CQaQb-heterocyclyl, CQaQb-bicyclic heterocyclyl, or CQaQb-aryl; R1 is CO2H, CQcQdCO2H, tetrazolyl, CH2tetrazolyl, CONR4R5, NR4CO2R6, NR4COR6 or 1,2,4triazol-3-yl (un)substituted on a ring C; or R1 = imidazolyl or pyrazolyl wherein optionally the imidazole or pyrazole ring is fused to give an (un) substituted bicyclic or tricyclic ring system; R2a and R2b = H, halo, CN, SO2alkyl, SR4 or NO2 or (un)substituted alkyl or (un)substituted alkoxy. R4 is H or (un) substituted alkyl; R5 is H or (un) substituted alkyl, aryl, heterocyclyl, SO2aryl, SO2alkyl, SO2heterocyclyl, CQaQbaryl, or CQaQbheterocyclyl; or R4 and R5 together with the N to which they are attached form a heterocyclic or bicyclic heterocyclic ring; R6 is (un)substituted alkyl or aryl; R7 is H, F or alkyl; R8 is H, hydroxy, F or alkyl; or R7 and R8

together with the C to which they are attached form a cycloalkyl ring, optionally containing up to one heteroatom = 0, S, NH and N-alkyl; or R7 and R together with the C to which they are attached form a carbonyl group; and Qa and Qb = H, CH3 and F; Qc and Qd = H and CH3; addnl. details including provisos are given in the claims.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 8 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 2006:1147677 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 145:471368

TITLE: Preparation of furan derivatives as human EP1 receptor

antagonists

INVENTOR(S): Bit, Rino Antonio; Giblin, Gerard Martin Paul;

Hall, Adrian; Hurst, David Nigel; Kilford, Ian

Reginald; Scoccitti, Tiziana Glaxo Group Limited, UK

PATENT ASSIGNEE(S): Glaxo Group Limited, USOURCE: PCT Int. Appl., 85pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patient

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT				KIN		DATE			APPL						ATE	
WO 2006																
	AE,															
						DE,										
						ID,										
						LT,										
						NZ,										
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RW:	AT,					CZ.	DE.	DK.	EE.	ES.	FI.	FR.	GB.	GR.	HU.	TE.
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						NA,										
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EP 1874							0109		EP 2	006-	7245	5.8		2	กกรก	424
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OTHER SOURCE	E(S):			MAR	PAT	145:	4713		WO Z	000-	mr J O	00		vi Z	0000	444

II

AB The title compds, with general formula I [wherein R1 = CO2H, imidazoly1, pyrazoly1, etc.; R2 = H or (un) substituted C1-3 alky1, R3 and R4 = independently H, halo, CN, etc.; R5 = (un) substituted C2-20 alky1, C2-20 alkeny1, C2-20 alkeny1, c2-20, S, SO, or SO2; Z = 0, S, SO, or SO2] or pharmaceutically acceptable derive. thereof are prepared as human EPI receptor antagonists. For example, compound II-Na was prepared in a multistep synthesis. II-Na exhibited a pICSO 2 8 in the binding assay test for human prostanoid EPI receptor using Chinese hamster ovary-K1 (CHO-K1) rells.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 9 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 2006:627600 ZCAPLUS Full-text

DOCUMENT NUMBER: 145:83231

TITLE: Pyridine compounds as selective EP1 antagonists, their preparation, pharmaceutical compositions, and use in

therapy

INVENTOR(S): Giblin, Gerard Martin Paul; Ball, Adrian; Hurst,

David Nigel; Rawlings, Derek Anthony; Scoccitti,

Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

		ENT :				KIN		DATE					TION				ATE	
						A1		2006	0629				-EP14				0051	221
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			CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML	, MF	, NE,	SN,	TD,	TG,	BW,	GH,
			GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ	, TZ	, UG,	ZM,	ZW,	AM,	ΑZ,	BY,
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													-3183					
													-2592					
	ΕP	1833	795			A1		2007	0919		ΕP	2005	-8177	67		2	0051	221
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		2007											-DN42					
													-7142					
													-7830					
													-3332				0070	
	CN	1011	2843	0		A		2008	0220				-8004				0070	
PRIOR	IT	APP	LN.	INFO	. :								-2826					
													-8458				0050	
													-2467				0051	
											WO	2005	-EP14	061		W 2	0051	221
OTHER	SC	DURCE	(S):			MAR	PAT	145:	8323	1								

OTHER SOURCE(S): MARPAT 145:83231

12

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The invention relates to pyridine compds. of formula I, which are antagonists AB of prostaglandin E2 receptors EP1 subtype. In compds. I, X is N and Y is CH or X is CH and Y is N: Z is O. S. SO. or SO2: R1 is carboxy. sulfonvlaminocarbonvl, carboxymethyl, acylamino, tetrazolyl, or tetrazolylmethyl; R2 and R3 are independently selected from H, halo, cyano, SH, nitro, alkylsulfonyl, (un)substituted alkylthio, (un)substituted alkyl, (un) substituted alkoxy, (un) substituted aryl, and (un) substituted heteroaryl; R4 and R5 are independently H, halo, NH2, (un)substituted alkyl, (un) substituted alkoxy, or primary or secondary amino; R6 is (un) substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted heterocyclyl-C(R9)(R10)-, or (un)substituted aryl-C(R9)(R10)-, where R9 and R10 are independently selected from H, Me, and F; R7 is H, F, or alkyl; and R8 is H, OH, F, or alkyl, or R7 and R8, together with the carbon atom to which they are attached, form a cycloalkyl ring, optionally containing one heteroatom selected from O, S, NH, and N-alkyl, or R7 and R8, together with the carbon atom to which they are attached, form a carbonyl group. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I together with a pharmaceutical carrier and/or excipient, as well as to the use of the compns, for the treatment of conditions mediated by the action of prostaglandin E2 at the EP1 receptor, such as pain, inflammatory disorders, or neurodegenerative disorders. Regioselective benzylation of 4-chloro-2-(hydroxymethyl)phenol followed by bromination, conversion to the organozinc reagent, substitution of Et 6-bromo-2-pyridinecarboxylate, and debenzylation gave pyridinecarboxylate II, which was benzylated with 4-chloro-2-fluorobenzyl bromide and hydrolyzed with NaOH to give sodium pyridinecarboxylate III. Of the compds. of the invention, 14 compds., e.g., III, expressed pIC50 values of 7.5 or higher for EP1 receptor binding and 13 compds., e.g., III, expressed pKi values of 7.5 or higher for antagonism of EP1 calcium mobilization.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 10 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 2006:315138 ZCAPLUS Full-text

DOCUMENT NUMBER: 144:480399

TITLE: Discovery of novel biaryl heterocyclic EP1 receptor

antagonists

AUTHOR(S): Hall, Adrian; Bit, Rino A.; Brown, Susan H.;

Chaignot, Helene M.; Chessell, Iain P.; Coleman, Tanya; Giblin, Gerard M. P.; Hurst, David N.; Kilford, Ian P.; Lewell, Xiao Q.; Michel, Anton D.;

Mohamed, Shiyam; Naylor, Alan; Novelli, Riccardo; Skinner, Lee; Spalding, David J.; Tang, Sac P.;

Wilson, Richard J.

CORPORATE SOURCE: Neurology and Gastrointestinal Centre of Excellence

for Drug Discovery, GlaxoSmithKline, Essex, CM19 5AW,

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(10), 2666-2671 CODEN: BMCLE8; ISSN: 0960-894X

CODEN: BRCLEO; 133N: 0900-894

PUBLISHER: Elsevier B.V. DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:480399

AB We describe the generation of novel EPI receptor antagonists by investigation of thiophene isosteres. In addition, we disclose preliminary in vitro and in vivo DMPK for selected commods.

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 11 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 11

ACCESSION NUMBER: 2005:1220712 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:477851

TITLE: Preparation of sodium 6-(2-bipheny1)-2-

pyridinecarboxylates for treating conditions mediated
by the action of PGE2 at the EP1 receptor

INVENTOR(S): Bit, Rino Antonio; Giblin, Gerard Martin Paul;

Hall, Adrian; Hayhow, Thomas; Hurst, David Nigel; Kilford, Ian Pegipald; Miller, Neil Derek; Naylor,

Alan; Novelli, Riccardo; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT	NO.			KIN	D	DATE			APPL	ICAT				D.	ATE	
WO	2005	1083	69		A1		2005	1117		WO 2	005-				2	0050	429
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		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,
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		SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,
		ZM,	ZW														
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		AZ,	BY,	KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
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		MR,	ΝE,	SN,	TD,	TG											
EP	1742	916			A1		2007	0117		EP 2	005-	7380	52		2	0050	429
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											RO,						
JP	2007	5363	09		T		2007	1213		JP 2	007-	5119	89		2	0050	429
US	2007	0225	340		A1		2007	0927		US 2	006-	5685	73			0061	
IORITY	APP	LN.	INFO	. :						GB 2	004-	1012	1		A 2	0040	506
										WO 2	005-	EP47:	26		W 2	0050	429
HER SC	URCE	(S):			MARI	PAT	143:	4778	51								

OTHER SOURCE(S): MARPAT 143:47785

AB The title compds. I [A = (un)substituted aryl, 5-6 membered heterocyclyl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = 0, S, S0, S02; R1 = CO2H, CN, COalkyl, etc.; R2a, R2b = H, halo, CN, etc.; Rx = (un)substituted alkyl [wherein 1 or 2 of the non-terminal carbon atoms are optionally replaced by NR4, 0 or S0n (wherein n = 0-2)], (un)substituted alkenyl, (un)substituted alkynyl, etc.; R8, R9 = H, halo, CF3, alkoxy, alkyl, useful in the treatment of conditions mediated by the action of PGE2 at the EP1 receptor (which is associated with smooth muscle contraction, pain (in particular inflammatory, neuropathic and visceral), inflammation, allergic activities, renal regulation and gastric or enteric mucus secretion), were prepared Thus, treating suspension of Et 6-(5'-bromo-2'-((2-methyl-2-propen-l-yl)oxyl-2-biphenylyl)-2-pyridinecarboxylate in EtcH with 1M NoOH afforded II. The exemplified compods. I showed an antagonist pIC50 of 6.0 or greater at EP2 receptors. The pharmaceutical composition comprising the compound I is disclosed.

pharmaceutical composition comprising the compound I is disclosed.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 12 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 12

ACCESSION NUMBER: 2005:523415 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:59814

TITLE: Preparation of aryl-substituted pyrroles as prostanoid

EP1 inhibitors useful for treating inflammation INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Healy,

Mark Patrick; Lewell, Xiao Qing; Miller, Neil Derek; Novelli, Riccardo; King, Francis David; Naylor, Alan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 78 pp.

CODEN: PIXXD2 Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

DOCUMENT TYPE:

PA:	TENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						_											
WO	2005	0541	91		A1		2005	0616		WO 2	004-	EP13	744		2	0041	130
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,
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AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 20060906 EP 2004-803473 EP 1697319 A1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS JP 2007513120 T 20070524 JP 2006-541906 20041130 US 2006-596153 20060913 GB 2003-28024 A 20031203 WO 2004-EP13744 W 20041130 US 20070072906 A1 20070329 US 2006-596153 PRIORITY APPLN. INFO.:

MARPAT 143:59814 OTHER SOURCE(S):

Title compds. I [A = aryl, heterocyclyl, etc.; B = Ph, pyridyl; Z = 0, SOO-2; AB R1 = carboxy, CN, alkoxy, etc.; R2a-2b = H, halo, alkyl, etc.; Rx = alkyl, etc.; R8 = H, C1, CF3, etc.; R9 = halo, H, CF3, alkyl] are prepared For instance, 6-[2-(5-Chloro-2-benzyloxyphenyl)-5-methylpyrrol-1- yl]picolinic is prepared via the metalation/carboxylation of 6-[2-(5-chloro-2benzyloxyphenyl)-5-methylpyrrol-1-yl]-2-bromopyridine. Compds. of the invention have an antagonist pIC50 = 6.0 to 9.0 at EP1 receptors and pIC50 < 6.0 at EP3 receptors. I are useful in the treatment of inflammatory disorders.

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 13 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 13

ACCESSION NUMBER: 2005:395279 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:447210

TITLE: Preparation of heterocyclic compounds for treating conditions mediated by EP1 receptor and TxA2 receptor

Giblin, Gerard Martin Paul; Hall, Adrian; Hurst, INVENTOR(S): David Nigel; Lewell, Xiao Qing; Lorthioir, Olivier Eric; McKeown, Stephen Carl; Scoccitti, Tiziana;

Watson, Stephen Paul

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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WO 2005040128
                        A1 20050506
                                          WO 2004-EP11964
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
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            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
            SN, TD, TG
    EP 1675832
                         Α1
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                                          EP 2004-790757
                                                                  20041021
    EP 1675832
                         B1
                               20080220
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR
    JP 2007509104
                         т
                               20070412
                                          JP 2006-536056
                                           AT 2004-790757
    AT 386725
                         Т
                               20080315
                                                                  20041021
    US 20070060596
                               20070315
                                           US 2006-576460
                                                                  20060522
                         A1
PRIORITY APPLN. INFO.:
                                           GB 2003-24893
                                                              A 20031024
                                           GB 2003-24895
                                                              A 20031024
                                           WO 2004-EP11964
                                                             W 20041021
OTHER SOURCE(S):
                       CASREACT 142:447210; MARPAT 142:447210
GΙ
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$$\mathbb{R}^{2?} \xrightarrow{\mathbb{R}^{2}} \mathbb{R}^{8} \mathbb{R}^{9} \xrightarrow{\mathbb{N}^{-\mathbb{N}}} \mathbb{R}^{1}$$

AB Compds. of formula [wherein W, X = N or CR10 (wherein R10 = H, halogen, each (un) substituted alkyl, arvl, or heterocyclyl); Y = N or CR12 (wherein R12 = H, halogen, Me, CF3); Z = O, S, SO, SO2; R1 = CO2R4, CONR5R6, CH2CO2H, (un) substituted SO2alkyl, SO2NR5R6, NR5CONR5R6, 2H-tetrazol-5-ylmethyl (un) substituted heterocyclyl; R2a, R2b = H, halo, each (un) substituted alkyl, alkoxy, or heteroaryl, cyano, SO2alkyl, SR5, NO2, CONR5R6; Rx = (un) substituted alkyl (wherein 1 or 2 of the nonterminal carbon atoms are optionally substituted by a group independently selected from NR4, O, S, SO, and SO2) or Rx = each (un)substituted COaOb-heterocyclyl, COaOb-bicyclic heterocyclyl, or CQaQb-aryl; R4, R5 = H, (un)substituted alkyl; R6 = H, cyano, each (un)substituted alkyl, heteroaryl, SO2aryl, SO2alkyl, SO2heteroaryl, CQaQbaryl, or CQaQbheteroaryl, COR7; R7 = H, each (un) substituted alkyl, heteroaryl, or aryl; R8, R9 = H, F, alkyl; or CR8R9 together forms a cycloalkyl ring, optionally containing up to one heteroatom selected from O, S, NH or N-alkyl; Qa, Qb = H, Me, F] or pharmaceutically acceptable derivs. thereof are prepared These compds. including pyrazole-3-carboxylic acids and pyrrole-3-carboxylic acids have activity at both the EP1 and TP receptors and are useful in the treatment of conditions such as inflammatory pain, neuropathic pain or visceral pain mediated by the action of prostaglandin E2 (PGE2) at the EP1 receptor and conditions mediated by the action of thromboxane on the TP (also known as TxA2) receptor. Thus, Me 1H-pyrazole-3carboxylate (12.61 mg, 0.1 mmol) was dissolved in a 0.105 M solution of potassium tert-butoxide in ethanol (1 mL, 11.78 mg, 0.105 mmol), stirred at room temperature for 5 min, treated with a 0.1 M solution of 4-bromo-2-

(bromomethyl) phenyl phenylmethyl ether in ethanol (1 mL, 35.6 mg, 0.1 mmol), and stirred and heated at 60° under nitrogen for 4 h to give, after workup, 27.6% 1-[[5-bromo-2- [(phenylmethyl)oxy]phenyl]methyl]-5-methyl-1H-pyrazole-3carboxylic acid. The compds. I had an antagonist binding pIC50 value of 6.2-9.9 at human EP1 receptors and a pIC50 value of <5.7 at human EP3 receptors and exhibited a functional pKi of 6.2-10.5 and/or a functional pIC50 of 5.3-8.9.

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 14 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 14

ACCESSION NUMBER: 2005:371224 ZCAPLUS Full-text

13

DOCUMENT NUMBER: 142:430147

TITLE: Preparation of cyclohexene compounds which bind with

high affinity to the EP1 receptor

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Hurst,

David Nigel PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 54 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

OTH GI

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	20050				A1		2005	0428					365		2	0041	006
							AU,										
							DE,										
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							PL,										
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	RW:						MW.										
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EP :	1670				A1		2006	0621		EP 2	004-	7902	67		2	0041	006
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							RO,										
JP :	20075																006
PRIORITY	APPI	N.	INFO	. :						GB 2	003-	2358	4		A 2	0031	008
										WO 2	004-1	EP11:	365	1	W 2	0041	006
OTHER SOU	JRCE	(S):			CASI	REAC	T 14	2:43	0147	; MAI	RPAT	142	:430	147			

$$\mathbb{R}^{22}$$
 \mathbb{R}^{8}
 \mathbb{R}^{9}
 \mathbb{R}^{1}
 \mathbb{R}^{21}
 \mathbb{R}^{3}
 \mathbb{R}^{9}
 \mathbb{R}^{1}
 \mathbb{R}^{1}

AB The title compds. I [A = (un)substituted aryl, 5-6 membered heterocyclyl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = 0, S, S, S0; R1 = CO2H, CN, CH2CO2H, etc.; R21, R22 = H, halo, alkyl, etc.; R3 = (un)substituted alkyl (wherein 1 or 2 of the non-terminal carbon atoms are optionally substituted by (un)substituted NH, O, S, SO, SO2), alkenyl, etc.; R8, R9 = H, Cl, F, CF3, alkoxy, alkyll, useful in the treatment of conditions mediated by the action of PGE2 at EP1 receptors, were prepared E.g., a multi-step synthesis of II, was given. The compds. I had an antagonist pIC50 value of 6.5 to 9.5 at EP1 receptors and pICS0 of < 6.0 at EP3 receptors. The pharmaceutical composition comprising the compound I is disclosed.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 15 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 15

ACCESSION NUMBER: 2005:371223 ZCAPLUS Full-text

3

DOCUMENT NUMBER: 142:430146

TITLE: Preparation of cyclopentene compounds which bind with

high affinity to the EP1 receptor

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Hurst,
David Nigel; Kilford, Jan Reginald; Lewell, Xiao

Qing; Naylor, Alan; Novelli, Riccardo

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 201 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT :				KIN		DATE						NO.		D	ATE	
WO	2005				A1										2	0041	006
								AZ,									
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		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
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		AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	TG													
EP	1670	763			A1		2006	0621		EP 2	004-	7659	25		2	0041	006
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	HR	
JP	2007	5090	39		T		2007	0412		JP 2	006-	5301	39		2	0041	006
PRIORIT	Y APP	LN.	INFO	. :						GB 2	003-	2358	1	- 2	A 2	0031	800
										WO 2	004-1	EP11	364	1	W 2	0041	006
OTHER S	OURCE	(S):			CAS	REAC	T 14	2:43	0146	; MAI	RPAT	142	:430	146			

19

$$\mathbb{R}^{22}$$
 \mathbb{R}^{21}
 \mathbb{R}^{3}
 \mathbb{R}^{3}
 \mathbb{R}^{3}
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 \mathbb{R}^{3}
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 \mathbb{R}^{3}
 \mathbb{R}^{3}

AB The title compds. I [A = (un)substituted aryl, 5-6 membered heterocyclyl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = O, S, SO, SO2; R1 = CO2H, CN, CH2CO2H, etc.; R21, R22 = H, halo, alkyl, etc.; R3 = (un)substituted alkyl (wherein 1 or 2 of the non-terminal carbon atoms are optionally substituted by (un)substituted NH, O, S, SO, SO2), alkenyl, etc.; R8, R9 = H, Cl, F, CF3, alkoxy, alkyll, useful in the treatment of conditions mediated by the action of PGE2 at EPI receptors, were prepared Thus, hydrolysis of (2,4-dichlorophenyl)methyl 6-{2-[2-{[(2,4-dichlorophenyl)methyl]oxy)-5-(trifluoromethyl)phenyl]-1-cyclopenten-1-yl)- 2-pyridinecarboxylate with 2M NaOH solution afforded II. The compds. I had an antagonist pICSO value of 6.0 to 9.5 at EPI receptors. The pharmaceutical composition comprising the compound I is disclosed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 16 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 16

ACCESSION NUMBER: 2005:371217 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:430145

TITLE: Preparation of heterocyclyl compounds which bind with

high affinity to the EP1 receptor
INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Ac

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Kilford, Jan Reginald; Lewell, Xiao Qing; Miller,

Meil Derek; Naylor, Alan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 67 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT I	MO.			KIN	D	DATE			APPL	ICAT:	ION I	MO.		D	ATE	
wo.	2005				A1	-	2005	0428		WO 2			366		2	0041	
	W:						AU,								_		
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		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI
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		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
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		SN,	TD,	TG													
EP	1670	756			A1		2006	0621		EP 2	004-	7659:	26		2	0041	006

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR JP 2007508267 Т 20070405 JP 2006-530141 PRIORITY APPLN. INFO.: GB 2003-23585 A 20031008

WO 2004-EP11366 OTHER SOURCE(S): CASREACT 142:430145; MARPAT 142:430145

W 20041006

The title compds. I [A = (un)substituted arvl, 5-6 membered heterocyclyl, AB bicyclic heterocyclyl; B = Ph, pyridyl; D = (un)substituted 5-6 membered heterocyclyl ring containing one or two heteroatoms selected from N. S and O (wherein X and Y are selected from N and C); Z = O, S, SO, SO2; R1 = CO2H, CN, CH2CO2H, etc.; R21, R22 = H, halo, alkyl, etc.; R3 = (un)substituted alkyl (wherein 1 or 2 of the non-terminal carbon atoms are optionally substituted by (un) substituted NH, O, S, SO, SO2), alkenyl, etc.], useful in the treatment of conditions mediated by the action of PGE2 at EP1 receptors, were prepared Thus, heating Me 3-(4-oxopentanoy1)benzoate with 2-benzyloxyaniline. HCl at $120\,^{\circ}\mathrm{C}$ for 24 h followed by hydrolysis of the resulting ester with 2M NaOH afforded the benzoic acid II. The compds. I had an antagonist pIC50 value of > 6.0 at EP1 receptors and pIC50 of < 6.0 at EP3 receptors. The

pharmaceutical composition comprising the compound I is disclosed. REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 17 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 17

ACCESSION NUMBER: 2004:799566 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:314325

TITLE: Preparation of 3-(imidazol-1-v1)benzoic acid

derivatives for the treatment of conditions mediated

by the action of PGE2 at EP1 receptors

Giblin, Gerard Martin Paul; Hall, Adrian; Lewell,

Xiao Qing; Miller, Neil Derek

Glaxo Group Limited, UK

PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 36 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION: DATEME NO

INVENTOR(S):

PAT	CENT	NO.			KIN)	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-									-		
WO	2004	10831	85		A2		2004	0930		WO 2	004-	EP28	31		2	0040	317
WO	WO 2004083185				A3		2004	1104									
	W:	AE.	AG	AL.	AM.	AT.	AII.	A7.	BA.	BB.	BG.	BR.	BW.	BY.	BZ.	CA	CH

CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK. TR. BF. BJ. CF. CG. CI. CM. GA. GN. GO. GW. ML. MR. NE. SN. TD, TG

PRIORITY APPLN. INFO.: OTHER SOURCE(S):

GB 2003-6329 A 20030319 CASREACT 141:314325; MARPAT 141:314325

AB The title compds. [I; A = (un)substituted aryl, 5-6 membered heterocyclyl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = 0, S, SO, SO2; R1 = CN, alkyl, COalkyl, SO2alkyl, etc.; R21, R22 = H, halo, alkyl, alkoxy, etc.; R3 = alkyl wherein 1 or 2 of the non-terminal carbon atoms are optionally replaced by NH, N(alkyl), O, and SOn; n = 0-2; either Q = C and T = N; or Q = N and T = C; R8, R9 = H, halo, alkyl, CF3; with provisol, were prepared E.g., a 2-step synthesis of 3-[5-(2-benzyloxyphenyl)imidazol-1-yl]benzoic acid, starting from 2-benzyloxybenzaldehyde, Et 3-aminobenzoate and tosylmethyl isocyanide, was given. The exemplified compds. I had an antagonist pIC50 value of between 7.0 and 9.5 at EP1 receptors and pIC50 value of <6.0 at EP3 receptors. The pharmaceutical composition comprising the compound I is claimed.

L49 ANSWER 18 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 18 ACCESSION NUMBER: 2004:390204 ZCAPLUS Full-text

140:406635

DOCUMENT NUMBER:

TITLE: Preparation of benzoic acids and related compounds as

EP1 receptor antagonists for the treatment of prostaglandin mediated diseases.

INVENTOR(S):

Bit, Rino Antonio; Giblin, Gerard Martin Paul;

Hall, Adrian; Hurst, David Nigel; Kilford, Ian Reginald; Miller, Neil Derek; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.	KIN	D	DATE			APPL	ICAT	DATE								
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WO 200	WO 2004039753					20040513 WO 2003-EP12181								20031030			
WO 2004	WO 2004039753					2004	0715										
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             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                               20040525
                                          AU 2003-287979
     AU 2003287979
                         A1
                                                                  20031030
     EP 1556330
                         A2
                                20050727
                                          EP 2003-779828
                                                                  20031030
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                         A1
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                                                                  20050428
PRIORITY APPLN. INFO .:
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                                                               A 20021101
                                           WO 2003-EP12181
                                                              W 20031030
                       MARPAT 140:406635
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OTHER SOURCE(S):

Ι

AB Title compds. I [A = (un)substituted aryl, 5 or 6-membered heterocyclyl ring, bicyclic heterocyclyl; B = Ph, pyridyl; Z = O, S, SO, etc.; R1 = CO2R4, CN, CONR5R6, etc.; R2a, R2b = H, halogen, (un)substituted alkyl, etc.; Rx = (un) substituted alkyl, CQaQb-heterocyclyl, CQaQb-bicyclic heterocyclyl, etc.; R4, R5 = H, (un)substituted alkyl; R6 = H, (un)substituted alkyl, heteroaryl, etc.; R8, R9 = H, C1, F, etc.; Qa, Qb = H, CH3] and their pharmaceutically acceptable derivs, were prepared For example, the Suzuki coupling of Et 2'bromobiphenyl-3-carboxylate and 2-benzyloxy-5-chlorophenylboronic acid, e.g., prepared from 3-ethoxycarbonylphenylboronic acid, followed by hydrolysis afforded compound I [A-R1 = 3-carboxyphenyl; Z = 0; R2a = H, R2b = 5-C1; R8, R9 = H] in 39% overall yield. In human prostanoid EP1 receptor binding assays, 90-examples of compds. I exhibited pIC50 values ranging from 6.0->9.0 at the EP1 receptor and pIC50 values of <6.0 at the EP3 receptor. Of note, no toxicol. effects are indicated/expected (sic) when the compds. I are administered at the assay concentration of 3 nM. Compds. I are claimed useful for the treatment of prostaglandin mediated diseases, e.g., inflammation, pain, etc.

L49 ANSWER 19 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 19 ACCESSION NUMBER: 2003:972053 ZCAPLUS Full-text DOCUMENT NUMBER: 140:27757 TITLE: Preparation of pyrroles for the treatment of prostaglandin mediated diseases INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Healy,

SOURCE:

Mark Patrick; Lewell, Xiao Qing; Miller, Neil Derek;

Novelli, Riccardo

Glaxo Group Limited, UK PCT Int. Appl., 275 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT ASSIGNEE(S):

PAT	ENT :	NO.			KIN	D	DATE			APPL	ICAT	DATE					
WO	2003	 1019	 59	A1 20031211					 WO 2	003-	EP57	90		2	0030	530	
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		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW					
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		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
AU	2003	2384	55		A1		2003	1219		AU 2	003-		20030530				
EP	1509	499			A1		2005	0302		EP 2	003-		20030530				
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
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JP	2005	5323	47		T		2005	1027		JP 2	004-	5096	53		2	0030	530
US	2007	0082	912		A1		2007	0412		US 2	004-	5162	30		2	0041	129
IORITY APPLN. INFO.:										GB 2	002-	1278	5		A 2	0020	531
										WO 2	003-	EP57	90		W 2	0030	530
HER SC	URCE	(S):			MAR	PAT	140:	2775	7								

AB The title compds. [I; A = (un)substituted aryl, 5-6 membered heterocyclyl, biocyclic heterocyclyl; R1 = CO2H, CN, CH2CO2H, alkyl, etc.; R2, R3 = H, halo, alkyl, alkoxy, etc.; R4 = (un)substituted alkyl wherein 1 or 2 of the non-terminal carbon atoms may optionally be replaced by a O, (un)substituted NH, SOn (n = 0-2); R5, R6 = H, CF3, alkyl which bind with high affinity to the EP1 receptore, and are useful in medicine, in particular in the treatment of prostaglandin mediated diseases such as pain, inflammatory, immunol, bone, neurodegenerative or renal disorder, were prepared Preparation of 394 compds. I is described in detail. E.g., a 3-step synthesis of 3-[2-(2-benzyloxyphenyl)-5-methylpyrrol-1-yl]benzoic acid (starting from 2-benzyloxybenzaldehyde and Me vinyl ketone), was given. The exemplified compds. I had an antagonist pIC50 of 7.0-9.5 at EP1 receptors and pIC50 of <

6.0 at EP3 receptors. The pharmaceutical composition comprising the title compound I is claimed.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 20 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 20

ACCESSION NUMBER: 2003:818387 ZCAPLUS Full-text

DOCUMENT NUMBER: 139:323536

TITLE: Preparation of [2-(2-alkoxyphenyl)cyclopent-1-enyl] substituted (hetero)aromatic carboxylic acids with

high affinity to the EP1 receptor

INVENTOR(S): Giblin, Gerard Martin Paul; Hall, Adrian; Burst,

David Nigel; Kilford, Ian Reginald; Lewell, Xiao

Qing; Naylor, Alan; Novelli, Riccardo PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 180 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT	NO.		KIND DATE					API	PLICA		DATE							
WO	WO 2003084917						A1 20031016			WO	2003	-EP36		20030407					
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		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	M	I, MW	, MX,	MZ,	NO,	NZ,	OM,	PH,		
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SE	, SL	, TJ,	TM,	TN,	TR,	TT,	TZ,		
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		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BO	CH	, CY,	CZ,	DE,	DK,	EE,	ES,		
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		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GÇ	Q, GW	, ML,	MR,	NE,	SN,	TD,	TG		
CA	2481	035			A1		2003	1016		CA	2003	-2481	035		2	0030	407		
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EP	1492	757			A1		2005	0105		EP	2003	-7121		2	0030	407			
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BR	2003	0090	14		A		2005	0111		BR	2003		20030407						
					T 20050728								20030407						
CN	1659	131			A		2005	0824		CN	2003	-8125	87		20030407				
ZA	2004	0071	05		A		2006	0726		ZA	2004	-7105			2	0040	906		
US	2005	0239					2005	1027		US	2004	-5087	61		2	0040	922		
	7232				B2		2007	0619											
MX	2004	PA09	800		A		2004	1213		MX	2004	-PA98	00		2	0041	007		
NO	2004	0046	89		A		2004	1029		ИО	2004	-4689			2	0041	029		
IORIT	Y APP	LN.	INFO	. :								-8045				0020	408		
										GB	2003	-2881			A 2	0030	207		
							WO	2003	-EP36	61		W 2	0030	407					
THER S	HER SOURCE(S):						139:	3235	36										

OTHER SOURCE(S): MARPAT 139:323536

GI

The title compds. [I; A = (un) substituted Ph, 5-6 membered heterocyclyl, AB bicyclic heterocyclyl; R1 = CO2R4, CONR5R6, CH2CO2R4, alkyl, etc.; R2 = halo, alkyl, CN, etc.; R3 = alkyl wherein 1 or 2 of the non-terminal carbon atoms may optionally be replaced by NR4, O, SOn (n = 0-2), etc.; R4, R5 = H, alkyl; R6 = H, alkyl, SO2aryl, etc.; R8, R9 = H, alkyl; n = 0-2], useful for treating condition which is mediated by the action of PGE2 at EP1 receptors, were prepared E.g., a multi-step synthesis of [2-(5-chloro-2-

benzyloxyphenyl)cyclopent-1-enyl|benzoic acid (starting from 1.2dibromocyclopentene and (3-ethoxycarbonylphenyl)boronic acid), was given. The compds. I had an antagonist pIC50 value of between 7.0 and 9.5 at EP1 receptors and pIC50 value of <6.0 at EP3 receptors. Pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 21 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:69949 ZCAPLUS Full-text

2

DOCUMENT NUMBER: 148:168572

Indole derivatives as EP1 ligands, their preparation, TITLE:

pharmaceutical compositions, and use in therapy INVENTOR(S):

Hall, Adrian; Hurst, David Nigel; Scoccitti, Tiziana; Theobald, Pamela Joan

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 63pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO.						KIND DATE			APPL	ICAT:		DATE					
WO	TO 2008006793					A1 2008011			1	WO 2	007-	EP56	942	20070709				
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		GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	
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		IS,	ΙT,	LT,	LU,	LV,	MC,	MΤ,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	
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PRIORITY		GB 2006-14070							0	A 20060714								
OTHER SC	MARPAT 148:168572																	

GI

OTHER SOURCE(S):

26

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The invention relates to indole derivs. of formula I, which are ligands for the prostanoid EP1 receptor. In compds. I, R1 is CF3, C1, or Br; R2 is iso-Pr, iso-Bu, or 3,3-dimethylbutyl; R3 is substituted oxazolyl, substituted thiazolyl, or substituted thiazolylmethyl; and X is CH or N. The invention also relates to the preparation of I, pharmaceutical compns, comprising a compound I together with a pharmaceutical carrier and/or excipient, as well as to the use of the compns. for the treatment of conditions mediated by the action of prostaglandin E2 (PGE2) on the EP1 receptor, such as pain, inflammatory disorders, and neurodegenerative disorders. Acylation of 6chloroindole with isobutyryl chloride followed by hydride reduction and substitution of Et 2-bromothiazole-4-carboxylate resulted in the formation of N-thiazolylindole II, which underwent ester hydrolysis and amidation with 2aminobenzyl alc. to give N-(carbamovlthiazolyl)indole III. Several compds. of the invention, e.g., III, expressed pIC50 values above 7 for their affinity towards the prostanoid EP1 receptor and pKi values above 7.0 in a human EP1 calcium mobilization functional assay.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 22 OF 22 BIOSIS COPYRIGHT (c) 2008 The Thomson Corporation on STN

ACCESSION NUMBER: 2007:426422 BIOSIS Full-text

DOCUMENT NUMBER: PREV200700425637

TITLE: (2-((2-alkoxy)-phenyl) -cyclopent-lenyl) aromatic carbo and

heterocyclic acid and derivatives.

AUTHOR(S): Anonymous; Giblin, Gerard Martin Paul [Inventor]; Hall, Adrian [Inventor]; Hurst, David Nigel [Inventor];

Kilford, Ian Reginald [Inventor]; Lewell, Xiao Qing
[Inventor]; Naylor, Alan [Inventor]; Novelli, Riccardo

[Inventor]

CORPORATE SOURCE: Welwyn, United Kingdom

ASSIGNEE: Glaxo Group Limited

PATENT INFORMATION: US 07232821 20070619

SOURCE: Official Gazette of the United States Patent and Trademark

Office Patents, (JUN 19 2007)

CODEN: OGUPE7. ISSN: 0098-1133.

DOCUMENT TYPE: Patent

LANGUAGE: English

ENTRY DATE: Entered STN: 8 Aug 2007

Last Updated on STN: 8 Aug 2007

ABSTRACT: Compounds of formula (I) or a pharmaceutically acceptable derivative thereof: wherein A, R-1, R-2, R-x, R-8, R(9) and n are as defined in the

specification, a process for the preparation of such compounds, pharmaceutical compositions comprising such compounds and the use of such compounds in

medicine.

NAT. PATENT. CLASSIF.:514239500

CONCEPT CODE: Pathology - Therapy 12512

Pharmacology - General 22002

Pharmacology - Drug metabolism and metabolic stimulators

22003

INDEX TERMS: Major Concepts

Pharmacology

INDEX TERMS: Chemicals & Biochemicals

(2-((2-alkoxy)-phenyl)-cyclopent-lenyl) aromatic carbo derivatives: metabolic-drug; (2-((2-alkoxy)-phenyl)-cyclopent-lenyl) aromatic heterocyclic acid derivatives: metabolic-drug

=> file registry

FILE 'REGISTRY' ENTERED AT 10:30:20 ON 12 MAY 2008

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading Ll.str CF_{*} 13* 1 36----17 23* 5

chain nodes :

13 14 15 16 17 18 19 20 21 23 30 33 34 38 40 41 42 43 44 45 46 47 48 49 54 55

```
10/533036
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1 - 38 \quad 2 - 11 \quad 12 - 40 \quad 14 - 15 \quad 16 - 17 \quad 18 - 20 \quad 19 - 20 \quad 20 - 21 \quad 30 - 38 \quad 40 - 54 \quad 41 - 42 \quad 41 - 43
44-45 44-47 46-48 46-49 54-55
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-38 2-11 7-8 7-12 8-9 9-10 10-11 11-12 12-40 14-15 16-17 18-20 19-20
20-21 30-38 40-54 41-42 41-43 44-45 44-47 46-48 46-49 54-55
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2],[*3],[*4],[*5]
G2:C,N
G3:[*6],[*7]
G4:0,S
G5:[*8],[*9],[*10]
Connectivity:
21:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
23:Atom 30:CLASS 33:Atom 34:Atom 38:CLASS 40:CLASS 41:CLASS 42:CLASS
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45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 54:CLASS 55:CLASS

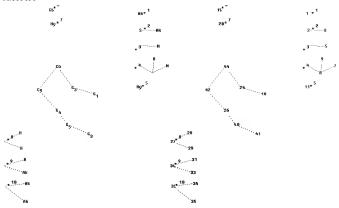
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Uploading L3.str

33: Saturation

43:CLASS 44:CLASS

Generic attributes :



chain nodes :

1 2 3 4 5 6 7 8 9 11 18 19 20 24 26 27 28 29 30 31 32 33 34 35 40 41 42 44

chain bonds :

2-3 4-5 6-8 7-8 8-9 18-24 24-44 26-40 26-42 27-28 27-29 30-31 30-33 32-34 32-35 40-41 42-44

exact/norm bonds :

2-3 4-5 6-8 7-8 8-9 18-24 24-44 26-40 26-42 27-28 27-29 30-31 30-33 32-34 32-35 40-41 42-44

G1:[*1],[*2],[*3],[*4],[*5]

G3:[*6],[*7]

G4:0,S

G5:[*8],[*9],[*10]

Connectivity:

9:1 E exact RC ring/chain 42:4 X maximum RC ring/chain 44:4 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:Atom 18:CLASS 19:Atom 20:Atom 24:CLASS 26:CLASS 27:CLASS 28:CLASS

29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS 34:CLASS 35:CLASS 40:CLASS 41:CLASS 42:Atom 44:Atom Generic attributes :

19: Saturation

: Unsaturated

42:

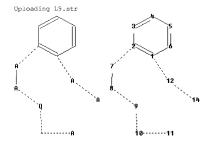
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Saturation
                        : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System
                       : Monocyclic
44:
Saturation
                         : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
Element Count :
Node 42: Limited
    C, C5-6
    N, NO-1
   S,SO
    0,00
    P,P0
Node 44: Limited
    C, C6
Uploading L4.str
                                                                23
chain nodes :
23
ring nodes :
1 \quad \bar{2} \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 10 \quad 11 \quad 12 \quad 13 \quad 14 \quad 15 \quad 16 \quad 17 \quad 18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-
15
15-16 16-17 17-18
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-
15
15-16 16-17 17-18
```

G1:[*1],[*2]

isolated ring systems : containing 1:7:13:

32

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 23:CLASS



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chain nodes:
9 10
ring nodes:
1 2 3 4 5 6 7 8 11 12 14
chain bonds:
1-12 2-7 8-9 9-10 10-11
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8 12-14
exact/norm bonds:
1-12 2-7 8-9 9-10 10-11 12-14
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8
isolated ring systems:
containing 1:
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Match level :

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=> d stat que L21 L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L3 $$\tt STR$$

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L4

G1







G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

L5 SCR 1841

L6 SCR 1946

L7 5110201 SEA FILE=REGISTRY ABB=ON PLU=ON 46.150.18/RID AND NRS>3

L9 STR



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L11 239 SEA FILE=REGISTRY SUB=L7 SSS FUL (L1 AND L3 AND L4 AND L9) AND
(L5 AND L6)

1.16

295 SEA FILE=REGISTRY ABB=ON PLU=ON (100-39-0/BI OR 100398-25-2/B I OR 1007-16-5/BI OR 107-82-4/BI OR 108-24-7/BI OR 121-43-7/BI OR 124-63-0/BI OR 13659-23-9/BI OR 136808-72-5/BI OR 137628-16-1/BI OR 14067-99-3/BI OR 141-43-5/BI OR 141-75-3/BI OR 150255-96-2/BI OR 176548-70-2/BI OR 179897-94-0/BI OR 188057-26 -3/BI OR 188815-32-9/BI OR 190661-29-1/BI OR 200956-32-7/BI OR 202409-82-3/BI OR 204841-19-0/BI OR 207115-22-8/BI OR 20986-40-7/BI OR 21190-88-5/BI OR 21739-93-5/BI OR 21856-53-1/BI OR 22921-67-1/BI OR 23915-07-3/BI OR 244205-40-1/BI OR 26628-22-8/ BI OR 353743-43-8/BI OR 363-24-6/BI OR 3637-61-4/BI OR 3731-52-0/BI OR 380430-56-8/BI OR 3808-91-1/BI OR 402-45-9/BI OR 41288-96-4/BI OR 4214-79-3/BI OR 4334-87-6/BI OR 459-46-1/BI OR 4635-59-0/BI OR 5419-55-6/BI OR 557-21-1/BI OR 583-53-9/BI OR 60-12-8/BI OR 612832-83-4/BI OR 612833-40-6/BI OR 612833-41-7/BI OR 612833-60-0/BI OR 612833-61-1/BI OR 612833-62-2/BI OR 612833-63-3/BI OR 612833-64-4/BI OR 612833-65-5/BI OR 612833-66 -6/BI OR 612833-67-7/BI OR 612833-68-8/BI OR 612833-69-9/BI OR 612833-70-2/BI OR 612833-71-3/BI OR 612833-72-4/BI OR 612833-73 -5/BI OR 6307-83-1/BI OR 690259-48-4/BI OR 690259-49-5/BI OR 690259-50-8/BI OR 690259-51-9/BI OR 690259-52-0/BI OR 690259-53 -1/BI OR 690259-54-2/BI OR 690259-55-3/BI OR 690259-56-4/BI OR 690259-57-5/BI OR 690259-58-6/BI OR 690259-59-7/BI OR 690259-60 -0/BI OR 690259-61-1/BI OR 690259-62-2/BI OR 690259-63-3/BI OR 690259-64-4/BI OR 690259-65-5/BI OR 690259-66-6/BI OR 690259-67 -7/BI OR 690259-68-8/BI OR 690259-69-9/BI OR 690259-70-2/BI OR 690259-71-3/BI OR 690259-72-4/BI OR 690259-73-5/BI OR 690259-74 -6/BI OR 690259-75-7/BI OR 690259-76-8/BI OR 690259-77-9/BI OR 690259-78-0/BI OR 690259-79-1/BI OR 690259-80-4/BI OR 690259-81 -5/BI OR 690259-82-6/BI OR 690259-83-7/BI OR 690259-84-8/BI OR 690259-85-9/BI OR

L20

151 SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND L16 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON L20

=> d ibib abs hitstr L21 1-3

L21 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:315138 ZCAPLUS Full-text DOCUMENT NUMBER: 144:480399

TITLE: Discovery of novel biaryl heterocyclic EP1 receptor

antagonists

AUTHOR(S): Hall, Adrian; Bit, Rino A.; Brown, Susan H.; Chaignot,

Helene M.; Chessell, Tain P.; Coleman, Tanya; Giblin, Gerard M. P.; Hurst, David N.; Kilford, Ian R.; Lewell, Xiao Q.; Michel, Anton D.; Mohamed, Shiyam; Naylor, Alan; Novelli, Riccardo; Skinner, Lee; Spalding, David J.; Tang, Sac P.; Wilson, Richard J.

CORPORATE SOURCE: Neurology and Gastrointestinal Centre of Excellence for Drug Discovery, GlaxoSmithKline, Essex, CM19 5AW,

UK

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(10), 2666-2671

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:480399

B We describe the generation of novel EP1 receptor antagonists by investigation of thiophene isosteres. In addition, we disclose preliminary in vitro and in vivo DMPK for selected compds.

T 690259-48-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Discovery of novel biaryl heterocyclic EP1 receptor antagonists)

RN 690259-48-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:1220712 ZCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 143:477851

TITLE: Preparation of sodium 6-(2-biphenyl)-2-

pyridinecarboxylates for treating conditions mediated

by the action of PGE2 at the EP1 receptor

INVENTOR(S): Bit, Rino Antonio; Giblin, Gerard Martin Paul; Hall, Adrian; Hayhow, Thomas; Hurst, David Nigel; Kilford, Ian Reginald; Miller, Neil Derek; Navlor, Alan;

Novelli, Riccardo; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT:

English

PATENT INFORMATION:

	PATENT NO.									APPLICATION NO.										
										WO 2005-EP4726										
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	KZ,		
			LC.	LK.	LR.	LS,	LT.	LU,	LV.	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,		
			NI.	NO.	NZ,	OM,	PG.	PH,	PL.	PT.	RO.	RU.	SC.	SD,	SE,	SG,	SK,	SL,		
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			ZM.				,			,										
		RW:	BW.	GH,	GM,	KE,	LS.	MW,	MZ.	NA.	SD,	SL,	SZ.	TZ,	UG.	ZM.	ZW.	AM.		
								RU,												
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	EP 1742916										EP 2	005-	7380	20050429						
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								PL, PT, RO, SE, SI, JP 2007-511989												
											US 2006-568573									
	IORITY APPLN. INFO.:					***		2001	052.	GB 2004-10121										
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Ρ GT

AB The title compds. I [A = (un)substituted arvl, 5-6 membered heterocyclvl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = O, S, SO, SO2; R1 = CO2H, CN, COalkyl, etc.; R2a, R2b = H, halo, CN, etc.; Rx = (un)substituted alkyl [wherein 1 or 2 of the non-terminal carbon atoms are optionally replaced by NR4, O or SOn (wherein n = 0-2)], (un)substituted alkenyl, (un)substituted alkynyl, etc.; R8, R9 = H, halo, CF3, alkoxy, alkyl], useful in the treatment of conditions mediated by the action of PGE2 at the EP1 receptor (which is associated with smooth muscle contraction, pain (in particular inflammatory, neuropathic and visceral), inflammation, allergic activities, renal regulation and gastric or enteric mucus secretion), were prepared Thus, treating suspension of Et 6-{5'-bromo-2'-[(2-methyl-2-propen-1-yl)oxy]-2-biphenylyl}-2-

pyridinecarboxylate in EtOH with 1M NaOH afforded II. The exemplified compds. I showed an antagonist pIC50 of 6.0 or greater at EP2 receptors. The pharmaceutical composition comprising the compound I is disclosed.

ΙT 590261-30-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of sodium 6-(2-biphenyl)-2-pyridinecarboxylates for treating conditions mediated by the action of PGE2 at the EP1 receptor)

RN 690261-30-4 ZCAPLUS

2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-CN 2-yl]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS 5 RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:390204 ZCAPLUS Full-text 140:406635

DOCUMENT NUMBER:

TITLE: Preparation of benzoic acids and related compounds as

EP1 receptor antagonists for the treatment of prostaglandin mediated diseases.

INVENTOR(S): Bit, Rino Antonio; Giblin, Gerard Martin Paul; Hall,

Adrian; Hurst, David Nigel; Kilford, Ian Reginald; Miller, Neil Derek; Scoccitti, Tiziana

Glaxo Group Limited, UK

PATENT ASSIGNEE(S): SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT :	NO.			KIN	D	DATE			APPLICATION NO.						DATE		
WO 2004039753 WO 2004039753					A2 20040513 A3 20040715				WO 2	003-	20031030							
	W: RW:	CO, GH, LR, OM, TN, BW,	CR, GM, LS, PG, TR, GH,	CU, HR, LT, PH, TT, GM,	CZ, HU, LU, PL, TZ, KE,	DE, ID, LV, PT, UA, LS,	AU, DK, IL, MA, RO, UG, MW, TJ,	DM, IN, MD, RU, US, MZ,	DZ, IS, MG, SC, UZ, SD,	EC, JP, MK, SD, VC, SL,	EE, KE, MN, SE, VN, SZ,	EG, KG, MW, SG, YU, TZ,	ES, KP, MX, SK, ZA, UG,	FI, KR, MZ, SL, ZM, ZM,	GB, KZ, NI, SY, ZW,	GD, LC, NO, TJ,	GE, LK, NZ, TM,	
							HU,											

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TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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                        A1
                              20040525
                                         AU 2003-287979
                                                                20031030
                        A2
                              20050727
                                         EP 2003-779828
                                                                20031030
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
    JP 2006504767
                        Т
                              20060209
                                          JP 2004-547644
                                                                20031030
    US 20060235057
                        A1
                               20061019
                                          US 2005-533036
                                                                20050428
PRIORITY APPLN. INFO.:
                                          GB 2002-25548
                                                             A 20021101
                                          WO 2003-EP12181
                                                            W 20031030
OTHER SOURCE(S):
                       MARPAT 140:406635
GI
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AB Title compds, I [A = (un)substituted arvl, 5 or 6-membered heterocyclyl ring, bicyclic heterocyclyl; B = Ph, pyridyl; Z = O, S, SO, etc.; R1 = CO2R4, CN, CONR5R6, etc.; R2a, R2b = H, halogen, (un)substituted alkyl, etc.; Rx = (un) substituted alkyl, CQaQb-heterocyclyl, CQaQb-bicyclic heterocyclyl, etc.; R4, R5 = H, (un) substituted alkyl; R6 = H, (un) substituted alkyl, heteroaryl, etc.; R8, R9 = H, C1, F, etc.; Qa, Qb = H, CH3] and their pharmaceutically acceptable derivs, were prepared For example, the Suzuki coupling of Et 2'bromobiphenyl-3-carboxylate and 2-benzyloxy-5-chlorophenylboronic acid, e.g., prepared from 3-ethoxycarbonylphenylboronic acid, followed by hydrolysis afforded compound I [A-R1 = 3-carboxyphenyl; Z = 0; R2a = H, R2b = 5-C1; R8, R9 = H] in 39% overall yield. In human prostancid EP1 receptor binding assays, 90-examples of compds. I exhibited pIC50 values ranging from 6.0->9.0 at the EP1 receptor and pIC50 values of <6.0 at the EP3 receptor. Of note, no toxicol. effects are indicated/expected (sic) when the compds. I are administered at the assay concentration of 3 nM. Compds. I are claimed useful for the treatment of prostaglandin mediated diseases, e.g., inflammation, pain, etc.

IT 690259-48-48 690259-49-89 690259-80-88 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98 690259-51-98-98 690259-51-98-98 690259-61-98 690259-61-98 690259-61-98 690259-61-98 690259-61-98 690259-61-98 690259-61-98 690259-61-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-78-98 690259-980259-98-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 6902598 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 690259-98 6902598 690259-98 690259-98 690259-98 690259 690259-98 690259-98 690259 690259-98 690259 690259 690259 690259 690259 690259 690259 6902

Ι

\$90259-98-1P 690259-99-P 690260-03-PP 590260-03-PP 590260-03-PP 590260-03-PP 690260-03-PP 690260

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoic acids and related compds. as EP1 receptor antagonists for the treatment of prostaglandin mediated diseases.) 690259-48-4 ZCAPLUS

RN 690259-49-5 ZCAPLUS CN [1,1':2',1''-Terphenyl]-3-acetic acid, 5''-chloro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

RN 690259-50-8 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-2-acetic acid, 5''-chloro-2''-(phenylmethoxy)(9C1) (CA INDEX NAME)

RN 690259-51-9 ZCAPLUS

RN 690259-52-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(acetylamino)-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-53-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxopropyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-54-2 ZCAPLUS

 $\texttt{CN} \qquad \texttt{[1,1':2',1''-Terpheny1]-3-carboxylic acid, 5''-chloro-5-[(2-methyl-1-met$

oxopropyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-55-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxobutyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-56-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(benzoylamino)-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-57-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(methylsulfonyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-58-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-amino-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-59-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxobutyl)amino]-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-60-0 ZCAPLUS

- RN 690259-61-1 ZCAPLUS

- RN 690259-62-2 ZCAPLUS

- RN 690259-63-3 ZCAPLUS

- RN 690259-64-4 ZCAPLUS

RN 690259-65-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5-(acetylamino)-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-66-6 ZCAPLUS

RN 690259-67-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

- RN 690259-68-8 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxamide, 5''-chloro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690259-69-9 ZCAPLUS
- CN 1H-Tetrazole, 5-[5''-chloro-2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-3yl]- (9CI) (CA INDEX NAME)

- RN 690259-70-2 ZCAPLUS

- RN 690259-71-3 ZCAPLUS
- CN Benzamide, N-[[2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-4-yl]sulfonyl](9CI) (CA INDEX NAME)

- RN 690259-72-4 ZCAPLUS
- CN Benzamide, 4-nitro-N-[[2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-4-yl]sulfonyl]- (9CI) (CA INDEX NAME)

- RN 690259-73-5 ZCAPLUS
- CN Acetamide, N-[[2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-3-yl]sulfonyl]- (9CI) (CA INDEX NAME)

- RN 690259-75-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-76-8 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(2,4-difluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-77-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4chlorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-78-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4-chloro-2fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-80-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-81-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(4-pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-82-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3-pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-84-8 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3-thienylmethoxyl- (901) (CA INDEX NAME)

RN 690259-85-9 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2-thienylmethoxy)- (9C1) (CA INDEX NAME)

RN 690259-91-7 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)-, monomethyl ester (9CI) (CA
INDEX NAME)

$$\begin{array}{c} \text{MeC-C} \\ \text{F}_3\text{C} \\ \end{array}$$

RN 690259-92-8 ZCAPLUS

RN 690259-93-9 ZCAPLUS

RN 690259-94-0 ZCAPLUS

CN

[1,1':2',1''Terphenyl]-2-carboxylic acid, 2''-[(2,4-difluorophenyl)methoxy]-4-[(1-oxopropyl)amino]-5''-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 690259-95-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-[(2-methyl-1-roxopropyl)amino]-5''-(trifluoromethyl)- (9C1) (CA INDEX NAME)

RN 690259-96-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(2-oxo-1-pyrrolidinyl)-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-97-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-98-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-[(2-methylpropyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-99-5 ZCAPLUS

CN 2-Pyrazinecarboxylic acid, 6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

RN 690260-00-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5[(1-oxopropyl)amino]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-01-6 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxopropyl)amino]-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-02-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4-fluorophenyl)methoxy]-5-[(1-oxopropyl)amino]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-03-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(methoxyacetyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-04-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[(2-thienylacetyl)amino]- (9CI) (CA INDEX NAME)

RN 690260-05-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[[(phenylmethoxy)acetyl]amino]- (9CI) (CA INDEX NAME)

RN 690260-06-1 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5-[[(l-acetyl-4piperidinyl)carbonyl]amino]-5''-chloro-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-07-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5'''-chloro-5[(phenylacetyl)amino]-2'''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-08-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5'''-chloro-5-[[(3,5-dimethyl-4isoxazolyl)carbonyl]amino]-2'''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-09-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(3-methyl-1-oxobutyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-10-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(aminoacetyl)amino]-5''chloro-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-11-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-[(1-oxopropyl)amino]-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-12-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-[(2-methyl-1-oxopropyl)amino]2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-13-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-[(2,4difluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-14-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-bromo-5-cyano-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-15-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-16-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(aminocarbonyl)-2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CO}_2\text{H} \\ \text{F}_3\text{C} \\ \text{C}_{\text{C}} \\ \text{C}_{\text{H}_2} \\ \end{array}$$

RN 690260-17-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-[((2-hydroxyethyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-18-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-[(3-pyridinylmethyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-19-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-20-9 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-fluorophenyl)methoxy][1,1'biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-21-0 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4-difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-22-1 ZCAPLUS
- CN 4-Pyridinecarboxylic acid, 2-[2'-[(4-fluorophenyl)methoxy]-5'- (trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-23-2 ZCAPLUS
- CN 2-Pyrazinecarboxylic acid, 3-amino-6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-24-3 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

- RN 690260-25-4 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(4-fluorophenyl)methoxyl-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-26-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4-difluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-27-6 ZCAPLUS

RN 690260-28-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-methyl-5''-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

- RN 690260-29-8 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690260-30-1 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-[(4-fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

- RN 690260-31-2 ZCAPLUS
- CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5''-fluoro- (9CI) (CA INDEX NAME)

RN 690260-32-3 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[5-chloro-2-(phenylmethoxy)-3pyridinyl]- (CA INDEX NAME)

RN 690260-33-4 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[6-chloro-3-(phenylmethoxy)-2pyridinyl]- (CA INDEX NAME)

RN 690260-34-5 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-amino-2'-[6-chloro-3-(phenylmethoxy)2-pyridinyl]- (CA INDEX NAME)

RN 690260-35-6 ZCAPLUS

CN 3-Pyridinecarboxylic acid, 5-[2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-(CA INDEX NAME)

- RN 690260-36-7 ZCAPLUS

- RN 690260-37-8 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 6-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- IT 690261-75-7
 - RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of benzoic acids and related compds. as EP1 receptor antaconists for the treatment of prostaglandin mediated diseases.)
- RN 690261-75-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(2,4-difluorophenyl)methoxyl-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

```
IT 690260-39-0P 690260-42-5P 690260-45-8P
    690260-47-0P 690260-49-2P 690260-50-5P
    690260-51-6P 690260-52-7P 690260-53-8P
     690260-54-9P 690260-55-0P 690260-57-2P
    690260-60-7P 690260-61-8P 690260-62-9P
    690360-63-0P 690260-64-1P 690260-65-3P
    690260-66-3P 690260-72-1P 690260-73-2P
    690260-74-3P 690260-75-4P 690260-77-6P
    690260-78-7P 690260-79-8P 690260-81-2P
    690260-82-3P 690261-01-9P 690261-06-4P
    690261-07-5P 690261-08-6P 690261-09-7P
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    690261-14-4P 690261-15-5P 690261-16-6P
    690261-17-7P 690261-18-8P 690261-19-9P
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    690261-42-8P 690261-44-0P 690261-45-1P
    690261-48-4P 690261-49-5P 690261-50-8P
    690261-52-0P 690261-55-3P 690261-56-4P
    690261-57-5P 690261-61-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of benzoic acids and related compds. as EP1 receptor
        antagonists for the treatment of prostaglandin mediated diseases.)
RN
    690260-39-0 ZCAPLUS
    [1,1':2',1''-Terphenvl]-3-carboxvlic acid, 5''-chloro-2''-(phenvlmethoxv)-
CN
     , ethyl ester (9CI) (CA INDEX NAME)
```

```
RN 690260-42-5 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3-acetic acid, 5''-chloro-2''-(phenylmethoxy)-,
ethyl ester (9C1) (CA INDEX NAME)
```

RN 690260-45-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-acetic acid, 5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-47-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-4-acetic acid, 5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-49-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-amino-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-50-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(acetylamino)-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-51-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxopropyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-52-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(2-methyl-1oxopropyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-53-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxobutyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-54-9 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(benzoylamino)-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-55-0 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[bis(methylsulfonyl)amino]-5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-57-2 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxobutyl)amino]-2''- (phenylmethoxy)-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-60-7 ZCAPLUS

N 690260-61-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5-fluoro-2''-(phenylmethoxy)-,
ethyl ester (9CI) (CA INDEX NAME)

RN 690260-62-9 ZCAPLUS

RN 690260-63-0 ZCAPLUS

RN 690260-64-1 ZCAPLUS

RN 690260-65-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5''-chloro-2''-(phenylmethoxy), ethyl ester (9CI) (CA INDEX NAME)

RN 690260-66-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-72-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4fluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-73-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(2,4-difluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-74-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4chlorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-75-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4-chloro-2-fluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-77-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-78-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(4-pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-79-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-81-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3thienylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-82-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2-thienylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-01-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5[((2-methylpropyl)manio]carbonyl]-5''-(trifluoromethyl)-, methyl ester
(9C1) (CA INDEX NAME)

RN 690261-06-4 ZCAPLUS

RN 690261-07-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-amino-2''-(phenylmethoxy)-,
methyl ester (9CI) (CA INDEX NAME)

RN 690261-08-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4difluorophenyl)methoxy]-5''-(trifluoromethyl)-, methyl ester (9C1) (CA
INDEX NAME)

RN 690261-09-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxyl-4-[(1-oxopropyl)amino]-5''-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-10-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-[(2-methyl-1-oxopropyl)amino]-5''-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-12-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-bromo-5-cyano-2''-(phenylmethoxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 690261-13-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-(phenylmethoxy)-5''(trifluoromethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 690261-14-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(2-oxo-1-pyrrolidinyl)-2''(phenylmethoxy)-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-15-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5''-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 690261-16-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxopropyl)amino]-2''(phenylmethoxy)-5''-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX
NAME)

RN 690261-17-7 ZCAPLUS

RN 690261-18-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5-[(1-coxopropyl)amino]-5''-(trifluoromethyl)-,
methyl ester (9C1) (CA INDEX NAME)

RN 690261-19-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5[(methoxyacetyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-20-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[(2-thienylacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-21-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[[(phenylmethoxy)acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-22-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[[(1-acetyl-4piperidinyl)carbonyl]amino]-5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9C1) (CA INDEX NAME)

RN 690261-23-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[[(3,5-dimethyl-4-isoxazolyl)carbonyl]amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-24-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(3-methyl-1oxobutyl)amino]-2''-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

- RN 690261-25-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[[[[(9H-fluoren-9ylmethoxy)carbonyl]amino]acetyl]amino]-2''-(phenylmethoxy)-, methyl ester

(9CI) (CA INDEX NAME)

RN 690261-26-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-[(1-oxopropyl)amino]-2''(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-27-9 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-2-carboxylic acid, 4-[(2-methyl-1-oxopropyl)amino]-2''-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-30-4 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-32-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-33-7 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4-difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-36-0 ZCAPLUS

CN 4-Pyridinecarboxylic acid, 2-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-37-1 ZCAPLUS

CN 2-Pyrazinecarboxylic acid, 3-amino-6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-40-6 ZCAPLUS

RN 690261-41-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-42-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4difluorophenyl)methoxy]-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA
INDEX NAME)

RN 690261-44-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-methyl-2''-(phenylmethoxy)-,
ethyl ester (9CI) (CA INDEX NAME)

RN 690261-45-1 ZCAPLUS

RN 690261-48-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-(phenylmethoxy), phenylmethyl ester (9CI) (CA INDEX NAME)

RN 690261-49-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-[(4fluorophenyl)methoxy]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 690261-50-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5''-fluoro-, (2,4-difluorophenyl)methyl ester
(9C1) (CA INDEX NAME)

RN 690261-52-0 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[5-chloro-2-(phenylmethoxy)-3pyridinyl]-, ethyl ester (CA INDEX NAME)

RN 690261-55-3 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[6-chloro-3-(phenylmethoxy)-2pyridinyl]-, ethyl ester (CA INDEX NAME)

RN 690261-56-4 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-amino-2'-[6-chloro-3-(phenylmethoxy)-2-pyridinyl]-, methyl ester (CA INDEX NAME)

RN 690261-57-5 ZCAPLUS

CN 3-Pyridinecarboxylic acid, 5-[2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-61-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4''-chloro-2''-(phenylmethoxy), ethyl ester (9CI) (CA INDEX NAME)

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http://www.cas.org/support/stngen/stndoc/properties.html

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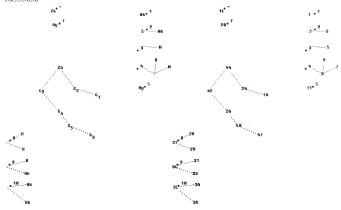
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10/533036
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1 - 38 \quad 2 - 11 \quad 12 - 40 \quad 14 - 15 \quad 16 - 17 \quad 18 - 20 \quad 19 - 20 \quad 20 - 21 \quad 30 - 38 \quad 40 - 54 \quad 41 - 42 \quad 41 - 43
44-45 44-47 46-48 46-49 54-55
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-38 2-11 7-8 7-12 8-9 9-10 10-11 11-12 12-40 14-15 16-17 18-20 19-20
20-21 30-38 40-54 41-42 41-43 44-45 44-47 46-48 46-49 54-55
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
G1:[*1],[*2],[*3],[*4],[*5]
G2:C,N
G3:[*6],[*7]
G4:0,S
G5:[*8],[*9],[*10]
Connectivity:
21:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
23:Atom 30:CLASS 33:Atom 34:Atom 38:CLASS 40:CLASS 41:CLASS 42:CLASS
43:CLASS 44:CLASS
45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 54:CLASS 55:CLASS
Generic attributes :
33:
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: Unsaturated

Uploading L3.str

Saturation



chain nodes :

chain bonds :

exact/norm bonds :

G1:[*1],[*2],[*3],[*4],[*5]

G3:[*6],[*7]

G4:0,S

G5:[*8],[*9],[*10]

Connectivity :

9:1 E exact RC ring/chain 42:4 X maximum RC ring/chain 44:4 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:Atom 19:CLASS 19:Atom 20:Atom 24:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 31:CLASS

32:CLASS 33:CLASS 34:CLASS 35:CLASS 40:CLASS 41:CLASS 42:Atom 44:Atom

Generic attributes : 19:

Saturation 42: : Unsaturated

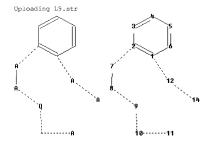
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Saturation
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Number of Carbon Atoms : less than 7
Type of Ring System
                     : Monocyclic
44:
Saturation
                      : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
Element Count :
Node 42: Limited
    C, C5-6
   N, NO-1
   S,SO
   0,00
   P,P0
Node 44: Limited
   C, C6
Uploading L4.str
                                                           23
chain nodes :
23
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G1:[*1],[*2]

93

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 23:CLASS



chain nodes:
9 10
ring nodes:
1 2 3 4 5 6 7 8 11 12 14
chain bonds:
1-12 2-7 8-9 9-10 10-11
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8 12-14
exact/norm bonds:
1-12 2-7 8-9 9-10 10-11 12-14
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8
isolated ring systems:
containing 1:

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 14:Atom

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=> d stat que L12 L1 STR

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L4 $\,$ STR $\,$

G1







G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

L5 SCR 1841

L6 SCR 1946

L7 5110201 SEA FILE=REGISTRY ABB=ON PLU=ON 46.150.18/RID AND NRS>3

L9 STR



Structure attributes must be viewed using STN Express query preparation.
Ll1 239 SEA FILE=REGISTRY SUB=L7 SSS FUL (L1 AND L3 AND L4 AND L9) AND
(L5 AND L6)

L12 9 SEA FILE=ZCAPLUS ABB=ON PLU=ON L11

=> file babs

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FILE COVERS 1980 TO DATE.

=> d stat que L48

L48 4 SEA FILE=BABS ABB=ON PLU=ON (6644860/BABSAN OR 6702500/BABSAN OR 6340976/BABSAN OR 6562995/BABSAN)

=> file beilstein

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FILE COVERS 1771 TO 2008.

*** FILE CONTAINS 10.322,808 SUBSTANCES ***

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* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.

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=> d stat que L47

L1 STR

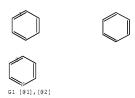
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. ${\tt L4}$

G1



Structure attributes must be viewed using STN Express query preparation. L9 $$\operatorname{\mathtt{STR}}$$



Structure attributes must be viewed using STN Express query preparation. L45 13 SEA FILE=BEILSTEIN SSS FUL (L1 AND L3 AND L4 AND L9) L46 9 SEA FILE=BEILSTEIN ABB=ON PLU=ON L45 AND BABSAN/FA L47 4 SEA FILE=BEILSTEIN ABB=ON PLU=ON L45 NOT L46

-> dup rem L12 L48 L47
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PROCESSING COMPLETED FOR L48

L50 13 DUP REM L12 L48 L47 (4 DUPLICATES REMOVED)
ANSWERS '1-9' FROM FILE ZCAPLUS

ANSWERS '10-13' FROM FILE BEILSTEIN -> d ibib abs hitstr L50 1-9; d ide allref L50 10-13

L50 ANSWER 1 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2007:743246 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:323038

PROCESSING COMPLETED FOR L47

CORPORATE SOURCE:

TITLE: Synthesis of Tetra-ortho-substituted,

Phosphorus-Containing and Carbonyl-Containing Biaryls

Department of Chemistry, Oregon State University,

Utilizing a Diels-Alder Approach

AUTHOR(S): Ashburn, Bradley O.; Carter, Rich G.; Zakharov, Lev N.

Corvallis, OR, 97331, USA

SOURCE: Journal of the American Chemical Society (2007),

129(29), 9109-9116

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:323038

The application of the Diels-Alder approach to biaryls (DAB) is described for the synthesis of tetra-ortho-substituted biaryl compds. containing orthogonally functionalized substituents. The syntheses of P-containing, disubstituted alkynes and carbonyl-containing, disubstituted alkynes were accomplished in two to three steps from com, available reagents. Subsequent Diels-Alder cycloaddns, with a range of oxygenated dienes yielded the target biaryls. Further functionalization through Pd-couplings is demonstrated on the P-containing biarvls. Selective manipulation of each of the remaining ortho substituents on the P-containing biaryls is demonstrated. One of these P-containing derivs. was used as a highly active catalyst for Suzuki coupling. For the carbonyl-containing series, a wide range of dienophile substituents were screened including esters, ketones, and amides. The key Diels-Alder cycloaddns, proceeded smoothly with the com, available 1-methoxy-1,3cyclohexadiene to yield the resultant tetra-ortho-substituted biaryls with excellent regioselectivity. The scope of the cycloaddn, process was also explored on the carbonyl-containing dienophiles with cyclic dienes. Acyclic dienes were also screened; however, they did not prove effective in the Diels-Alder process with the carbonyl-containing acetylenes. The ability to isolate enantiomerically pure biaryl atropisomers using a benzyl oxazolidinone is disclosed. Finally, the subsequent conversion to an axially chiral anilino alc. is also reported.

916978-88-6P 916978-92-2P 947612-43-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; preparation and Diels-Alder reaction of P-containing

and

carbonvl-containing alkynes with oxygenated dienes and cyclic dienes to give tetra-ortho-substituted biaryl compds.)

916978-88-6 ZCAPLUS RN

CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphino)-4''-methoxy-N.N.2.6-tetramethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

DM 916978-92-2 ZCAPLUS

Phosphine oxide, dicvclohexv1[4-methoxv-2'',6''-dimethv1-6'-nitro-6-CN (phenylmethoxy) [1,1':2',1''-terphenyl]-2-yl]- (CA INDEX NAME)

RN 947612-43-3 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3'-amine, 2''-(dicyclohexylphosphino)-4''-methoxy-N,N,2,6-tetramethyl-6''-(phenylmethoxy)-, hydrochloride (1:1) (CA INDEX NAME)

IT 947612-34-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and Diels-Alder reaction of P-containing and carbonylcontaining
alkynes with oxygenated dienes and cyclic dienes to give

tetra-ortho-substituted biaryl compds.)

RN 947612-34-2 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-3'-amine, 4''-methoxy-2,6-dimethyl-2''-(phenylmethoxy)- (CA INDEX NAME)

IT 916978-86-4P 916978-87-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and Diels-Alder reaction of P-containing and carbonyl-containing

alkynes with oxygenated dienes and cyclic dienes to give

tetra-ortho-substituted biaryl compds.)

RN 916978-86-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphinyl)-4''-methoxy2,6-dimethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

RN 916978-87-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphino)-4''-methoxy-2,6-dimethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

IT 947612-35-3P 947612-42-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and Diels-Alder reaction of P-containing and carbonyl-

containing
 alkynes with oxygenated dienes and cyclic dienes to give
 tetra-ortho-substituted biaryl compds.)

RN 947612-35-3 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3'-amine, 2''-(dicyclohexylphosphiny1)-4''-methoxy-N,N,2,6-tetramethy1-6''-(phenylmethoxy)- (CA INDEX NAME)

RN 947612-42-2 ZCAPLUS

CN Phosphine oxide, dicyclohexy1[4-methoxy-2''-methyl-6'-nitro-6-(phenylmethoxy)[1,1':2',1''-terphenyl]-2-yl]- (CA INDEX NAME)



REFERENCE COUNT:

SOURCE:

PUBLISHER:

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 2 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2006:1146810 ZCAPLUS <u>Full-text</u>

50

DOCUMENT NUMBER: 146:62815

TITLE: Diels-Alder approach to polysubstituted biaryls: rapid

entry to tri- and tetra-ortho-substituted

THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS

phosphorus-containing biaryls

AUTHOR(S): Ashburn, Bradley O.; Carter, Rich G.

CORPORATE SOURCE: Department of Chemistry, Oregon State University

(OSU), Corvallis, OR, 97331, USA

Angewandte Chemie, International Edition (2006), 45(40), 6737-6741

CODEN: ACIEF5; ISSN: 1433-7851

Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:62815

A Diels-Alder-based approach to the synthesis of highly functionalized biaryls from readily available precursors is disclosed. The utility of these biaryl templates in palladium-mediated couplings is explored along with subsequent redns. of the nitro and phosphine oxide moieties. Thus, Diels-Alder cycloaddn. of Me35iOC(OMe):CRHC(OMe):CRL with 2-Br-6-O2NC6H3C.tplbond.CP(O)R2 (R = cyclohexyl; preparation given) in PhNe in the presence of Et3N gave 2-Br-6-O2NC6H3C6H2-2-OH-4-ONE-6-PO)R2 (R = same). Finally, initial application of a synthesized biaryl as a highly active ligand in palladium-mediated coupling is carried out.

T 916978-88-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of tri- and tetra-ortho-substituted phosphorus-containing biarvls

via Diels-Alder approach to polysubstituted biaryls)

RN 916978-88-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphino)-4''-methoxy-N,N,2,6-tetramethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

- IT 916978-86-4P 916978-87-5P 916978-92-2P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (preparation of tri- and tetra-ortho-substituted phosphorus-containing biarvls $% \left(1\right) =\left(1\right) \left(1\right) \left($
- via Diels-Alder approach to polysubstituted biaryls)
- RN 916978-86-4 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphinyl)-4''-methoxy-2,6-dimethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

- RN 916978-87-5 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3'-amine, 2''-(dicyclohexylphosphino)-4''-methoxy-2,6-dimethyl-6''-(phenylmethoxy)- (CA INDEX NAME)

RN 916978-92-2 ZCAPLUS

CN Phosphine oxide, dicyclohexyl[4-methoxy-2'',6''-dimethyl-6'-nitro-6-(phenylmethoxy) [1,1':2',1''-terphenyl]-2-yl]- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 3 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3 ACCESSION NUMBER: 2006:315138 ZCAPLUS Full-text

DOCUMENT NUMBER: TITLE:

144:480399

70

Discovery of novel biaryl heterocyclic EP1 receptor

AUTHOR(S):

antagonists Hall, Adrian; Bit, Rino A.; Brown, Susan H.; Chaignot,

Helene M.; Chessell, Iain P.; Coleman, Tanya; Giblin,

Gerard M. P.; Hurst, David N.; Kilford, Ian R.; Lewell, Xiao Q.; Michel, Anton D.; Mohamed, Shiyam; Naylor, Alan; Novelli, Riccardo; Skinner, Lee; Spalding, David J.; Tang, Sac P.; Wilson, Richard J. Neurology and Gastrointestinal Centre of Excellence for Drug Discovery, GlaxoSmithKline, Essex, CM19 5AW,

CORPORATE SOURCE:

ПK Bioorganic & Medicinal Chemistry Letters (2006),

SOURCE:

16(10), 2666-2671

ΙT

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:480399

We describe the generation of novel EP1 receptor antagonists by investigation of thiophene isosteres. In addition, we disclose preliminary in vitro and in vivo DMPK for selected compds.

690259-48-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Discovery of novel biaryl heterocyclic EP1 receptor antagonists)

RN 690259-48-4 ZCAPLUS

[1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)-CN (9CI) (CA INDEX NAME)



REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 4 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2002:325630 ZCAPLUS Full-text

DOCUMENT NUMBER: 137:125038

TITLE: Total synthesis of the turrianes and evaluation of

their DNA-cleaving properties AUTHOR(S):

Furstner, Alois; Stelzer, Frank; Rumbo, Antonio; Krause, Helga

CORPORATE SOURCE: Max-Planck-Institut fur Kohlenforschung, Mulheim,

45470, Germany

Chemistry--A European Journal (2002), 8(8), 1856-1871

SOURCE: CODEN: CEUJED; ISSN: 0947-6539

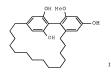
Wiley-VCH Verlag GmbH

PUBLISHER: DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:125038

GI



RN

The first total synthesis of three naturally occurring cyclophane derivs., e.g AB I, belonging to the turriane family of natural products is described. Their sterically hindered biaryl entity is formed by reaction of the Grignard reagent derived from an aryl bromide with an oxazoline derivative, and the macrocyclic tether of the targets is efficiently forged by ring closing metathesis. While conventional RCM catalyzed by the ruthenium-carbene complexes invariably leads to the formation of mixts. of both stereoisomers with the undesirable (E)-alkene prevailing, ring closing alkyne metathesis (RCAM) followed by Lindlar reduction of the resulting cycloalkynes opens a convenient and stereoselective entry into this class of compds. RCAM can either be accomplished by using the tungsten alkylidyne complex [(tBuO)3W.tplbond.CCMe3] or by means of a catalyst formed in situ from [Mo(CO)6] and para-trifluoromethylphenol. The latter method is significantly accelerated when carried out under microwave heating. Furthermore, the judicious choice of the protecting groups for the phenolic hydroxy functions turned out to be crucial. PMB-ethers were found to be compatible with the diverse reaction conditions en route to the targets; their cleavage, however, had to be carried out under carefully optimized conditions to minimize competing O-C PMB migration. The prepared turrianes are shown to be potent DNA cleaving agents under oxidative conditions when administered in the presence of copper ions. ΙT 444119-59-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis of the turrianes via a key ring closing alkyne metathesis cyclization and evaluation of their DNA-cleaving properties) 44419-59-9 ZCAPLUS

CN Oxazole, 2-[4'-[[[(1,1-dimethylethyl)diphenylsilyl]oxy]methyl]-6-methoxy2',4,6'-tris[(4-methoxyphenyl)methoxy][1,1'-biphenyl]-2-yl]-4,5-dihydro4,4-dimethyl- (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{CH2} \\ \text{Me} \\ \text{OMe} \\ \text{CH2} \\ \text{OMe} \\ \text{OMe}$$

IT 444119-77-1P 444119-78-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (total synthesis of the turrianes via a key ring closing alkyne

metathesis cyclization and evaluation of their DNA-cleaving properties)

RN 444119-77-1 ZCAPLUS

CN Oxazole, 2-[4'-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-methoxy2'',4,6'-tris[(4-methoxyphenyl]methoxy][1,1'-biphenyl]-2-yl]-4,5-dihydro4,4-dimethyl- (CA INDEX NAME)

RN 444119-78-2 ZCAPLUS

CN Oxazole, 2-[4'-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-methoxy-4-(methoxymethoxy)-2',6'-bis((4-methoxyphenyl)methoxy][1,1'-biphenyl]-2-yl]-4,5-dihydro-4,4-dimethyl- (CA INDEX NAME)

REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L50 ANSWER 5 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:234425 ZCAPLUS Fuil-text

DOCUMENT NUMBER: 148:426490

TITLE: Synthesis of Programmable Tetra-ortho-Substituted

SOURCE:

PUBLISHER:

Biaryl Compounds Using Diels-Alder

Cycloadditions/Cycloreversions of Disubstituted

Alkvnvl Stannanes

AUTHOR(S): Perkins, Johanna R.; Carter, Rich G. CORPORATE SOURCE:

Department of Chemistry, Oregon State University,

Corvallis, OR, 97331, USA

Journal of the American Chemical Society (2008),

130(11), 3290-3291

CODEN: JACSAT: ISSN: 0002-7863

American Chemical Society

Journal DOCUMENT TYPE:

Ι

LANGUAGE: English GI

AB Orthogonally functionalized, programmable biaryl templates, e.g., I, have been synthesized utilizing arvl acetylenic stannanes and oxygenated dienes in a cycloaddn./cycloreversion strategy. Sequential functionalization of each of the four ortho positions has been demonstrated. Subsequent resolution of a representative anilino phenol has been accomplished. Addnl., a highly active anhydrous, boroxin-based Suzuki coupling protocol has been developed for conversion of unreactive arvl chlorides.

1017280-76-0P 1017280-77-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of tetra-ortho-substituted biaryls via Diels-Alder cycloaddn. and cycloreversion of arylacetylenic stannanes with oxygenated dienes

followed by cross-coupling)

1017280-76-0 ZCAPLUS RN

CN INDEX NAME NOT YET ASSIGNED

RN 1017280-77-1 ZCAPLUS

CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 6 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:767247 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:522429

TITLE: Diels-Alder Approach for the Construction of

Halogenated, o-Nitro Biaryl Templates and Application to the Total Synthesis of the Anti-HIV Agent Siamenol

AUTHOR(S): Naffziger, Michael R.; Ashburn, Bradley O.; Perkins, Johanna R.; Carter, Rich G.

CORPORATE SOURCE: Department of Chemistry, Oregon State University,

Corvallis, OR, 97331, USA

SOURCE: Journal of Organic Chemistry (2007), 72(26), 9857-9865

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:522429

GT CASREACI 147:522429

- AB A rapid Diels-Alder approach to halogenated biaryl templates is described. These biaryl templates are available in two steps from the corresponding aromatic aldehydes. The scope of subsequent Suzuki couplings on the biaryl chlorides is explored. Good tolerance for both electron-donating and electron-withdrawing groups in the coupling process can be achieved. Further functionalization of the biaryl templates is described. Hydrogenation of the nitro moiety with concomitant removal of the benzyl ether yields the o-anilino, o-phenolic polyaryls. Selective reduction of the nitro group can be accomplished. Alternatively, the benzyl ether can be selectively removed under Lewis acidic conditions. The utilization of the Diels-Alder adducts for the synthesis of a series of chlorinated carbazoles via the Cadogan cyclization is also demonstrated. Finally, application of this technol. to the total synthesis of siamenol (I), an anti-HIV agent, is reported.
- IT 947513-91-9P 947513-94-2P 947513-96-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, functionalization and application to the synthesis of carbazoles and siamenol of biaryl templates via Diels-Alder reaction)

RN 947513-91-9 ZCAPLUS

CN 1,1':2',1''-Terphenyl, 4''-methoxy-2-methyl-3'-nitro-2''-(phenylmethoxy)(CA INDEX NAME)

RN 947513-94-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-4-carbonitrile, 4''-methoxy-3'-nitro-2''(phenylmethoxy)- (CA INDEX NAME)

RN 947513-96-4 ZCAPLUS

CN 1,1':2',1''-Terphenyl, 4''-methoxy-3'-nitro-2''-(phenylmethoxy)-3-(trifluoromethyl)- (CA INDEX NAME)

REFERENCE COUNT:

83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 7 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1220712 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:477851
TITLE: Preparation of sodium 6-(2-bipheny1)-2-

pyridinecarboxylates for treating conditions mediated

by the action of PGG2 at the EPI receptor

Bit, Rino Antonio; Giblin, Gerard Martin Paul; Hall,

Adrian; Hayhow, Thomas; Hurst, David Nigel; Kilford,

Ian Reginald; Miller, Neil Derek; Naylor, Alan;

Novelli, Riccardo; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE				
WO 2005108369	A1 20051117	WO 2005-EP4726	20050429				
W: AE, AG, AL	AM, AT, AU, AZ,	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,				
CN, CO, CR	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,				
GE, GH, GM	, HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KM, KP, KR, KZ,				
LC, LK, LR	LS, LT, LU, LV,	MA, MD, MG, MK, MN,	MW, MX, MZ, NA,				
NI, NO, NZ	OM, PG, PH, PL,	PT, RO, RU, SC, SD,	SE, SG, SK, SL,				
SM, SY, TJ	TM, TN, TR, TT,	TZ, UA, UG, US, UZ,	VC, VN, YU, ZA,				
ZM, ZW							
RW: BW, GH, GM	KE, LS, MW, MZ,	NA, SD, SL, SZ, TZ,	UG, ZM, ZW, AM,				
AZ, BY, KG	, KZ, MD, RU, TJ,	TM, AT, BE, BG, CH,	CY, CZ, DE, DK,				
EE, ES, FI	FR, GB, GR, HU,	IE, IS, IT, LT, LU,	MC, NL, PL, PT,				
RO, SE, SI	SK, TR, BF, BJ,	CF, CG, CI, CM, GA,	GN, GQ, GW, ML,				
MR, NE, SN	, TD, TG						
		EP 2005-738052					
		DK, EE, ES, FI, FR,					
		PL, PT, RO, SE, SI,					
		JP 2007-511989					
US 20070225340	A1 20070927	US 2006-568573					
PRIORITY APPLN. INFO.:		GB 2004-10121					
		WO 2005-EP4726	W 20050429				
OTHER SOURCE(S): GI	MARPAT 143:4778						

II

- AB The title compds. I [A = (un)substituted aryl, 5-6 membered heterocyclyl, bicyclic heterocyclyl; B = Ph, pyridyl; Z = O, S, SO, SO2; R1 = CO2H, CN, COalkyl, etc.; R2a, R2b = H, halo, CN, etc.; Rx = (un)substituted alkyl [wherein 1 or 2 of the non-terminal carbon atoms are optionally replaced by NR4, O or SOn (wherein n = 0-2)], (un)substituted alkynl, (un)substituted alkynyl, etc.; R8, R9 = H, halo, CP3, alkoxy, alkyl, useful in the treatment of conditions mediated by the action of PGG2 at the EP1 receptor (which is associated with smooth muscle contraction, pain (in particular inflammatory, neuropathic and visceral), inflammation, allergic activities, renal regulation and gastric or enteric mucus secretion), were prepared Thus, treating suspension of Et 6-[5'-bromo-2'-[(2-methyl-2-propen-1-yl)oxy]-2-biphenylyl-2-pyridinecarboxylate in EtcH with 1M NaOH afforded II. The exemplified compds. I showed an antagonist pICSO of 6.0 or greater at EP2 receptors. The pharmaceutical composition comporising the compound I is disclosed.
- IT 66949-15-0P 869496-16-1P 869496-17-2P 669499-16-3P 869495-16-3P 869499-2-2P 869499-23-0P 869499-23-0P 869499-23-0P 869499-21-8P 869499-22-3P 869499-23-0P 869499-36-5P 869499-32-5P 869499-36-5P 869499-36-3P 869499-37-3P 869499-37-3P 869499-37-3P 869499-37-3P 869499-37-3P 869499-37-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of sodium 6-(2-biphenyl)-2-pyridinecarboxylates for treating conditions mediated by the action of PGE2 at the EP1 receptor) 869499-15-0 ZCAPLUS

RN 869499-15-0 ZCAPLUS CN 2-Pyridinecarboxylic

2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- RN 869499-16-1 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(4-chloro-2fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-17-2 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2,4,5trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

● Na

RN 869499-18-3 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2-chloro-4fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

● Na

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2,3,6trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-20-7 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(4-chlorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-21-8 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2,6difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA
INDEX NAME)

Na

- RN 869499-22-9 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(tetrahydro-2furanyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- Na
- RN 869499-23-0 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[[4-(trifluoromethyl)phenyl]methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- RN 869499-24-1 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2,4difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA
 INDEX NAME)

- RN 869499-25-2 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(2,4,6trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- RN 869499-26-3 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(4-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- RN 869499-36-5 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(tetrahydro-3furanyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 869499-37-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-bromo-2'-[(tetrahydro-2H-pyran-4-y1)methoxy][1,1'-biphenyl]-2-y1]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 869499-39-8 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)



Na

RN 869499-40-1 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[[2-fluoro-4-(trifluoromethyl)phenyl]methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na

-

RN 869499-41-2 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chloro-6fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

● Na

RN 869499-42-3 ZCAPLUS

2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4,6-trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-45-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(tetrahydro-2-furanyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 869499-48-9 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chloro-4fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-49-0 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[2'-[(4-bromo-2-fluorophenyl)methoxy]-5'-chloro[1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-50-3 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-chloro-2fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na Na

RN 869499-51-4 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,6difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

RN 869499-52-5 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chlorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 869499-53-6 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(3,4,5trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 869499-54-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-6'-methyl-2''- (phenylmethoxy)-, sodium salt (9CI) (CA INDEX NAME)

A NI

- RN 869499-73-0 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(3-cyclopenten-1ylmethoxy)[1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

- Na
- RN 869499-74-1 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(1-cyclopenten-1ylmethoxy)[1,1'-biphenyl]-2-yl]-, sodium salt (1:1) (CA INDEX NAME)

● Na

- IT 690261-30-4P 869499-91-2P 869499-92-3P 869499-93-4P 869499-94-5P 869499-95-6P
 - 869499-96-7P 869499-97-3P 869499-98-9P
 - 869499-99-0P 869500-00-5P 869500-04-9P
 - 869500-09-4P 869500-16-3P 869500-17-4P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation of sodium 6-(2-biphenyl)-2-pyridinecarboxylates for treating conditions mediated by the action of PGE2 at the EP1 receptor)
- RN 690261-30-4 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-91-2 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-92-3 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[[2-fluoro-4-(trifluoromethyl)phenyl]methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-93-4 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chloro-6-fluorophenyl)methoxy][1,1'-biphenyl]-2-vl]-, ethyl ester (CA INDEX NAME)

CN

RN 869499-94-5 ZCAPLUS

2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4,6-trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-95-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chloro-4-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-96-7 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[2'-[(4-bromo-2-fluorophenyl)methoxy]-5'-chloro[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-97-8 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-chloro-2-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-98-9 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,6difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869499-99-0 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2-chlorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

CN

RN 869500-00-5 ZCAPLUS

2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(3,4,5-trifluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869500-04-9 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(tetrahydro-2furanyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869500-09-4 ZCAPLUS

RN 869500-16-3 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(1-cyclopenten-1-ylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 869500-17-4 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(3-cyclopenten-1-ylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L50 ANSWER 8 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:390204 ZCAPLUS Full-text

ACCESSION NUMBER: 2004:390204 DOCUMENT NUMBER: 140:406635

TITLE: Preparation of benzoic acids and related compounds as

EP1 receptor antagonists for the treatment of

prostaglandin mediated diseases.

INVENTOR(S): Bit, Rino Antonio; Giblin, Gerard Martin Paul; Hall,

Adrian; Hurst, David Nigel; Kilford, Ian Reginald;

Miller, Neil Derek; Scoccitti, Tiziana

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 96 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.				KIND DATE			APPLICATION NO.										
WO								WO 2003-EP12181										
WO										DD.	D.C.	DD.	DV	D.F.	0.7	011	ON	
	w:						AU,											
							DK,											
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	
		TN.	TR.	TT.	TZ.	UA.	UG,	US.	UZ.	VC.	VN.	YU.	ZA.	ZM.	ZW			
	RW:						MW,									AM.	A7.	
							TJ,											
							HU,											
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							CI,											16
	2003287979						AU 2003-287979											
EP	1556330		A2 20050727			EP 2003-779828					20031030							
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK		
JP				T 20060209				JP 2004-547644										
IIS	2006	0235	057		A1		2006	1019		IIS 2	005-	5330	36		2	0050	428	
	US 20060235057 ORITY APPLN. INFO.:				2000	1015			002-									
LUKII.	I MEE	LIN.	TIME															
										WU Z	003-	EP12	191		w 2	0031	030	
HER SO	DURCE	(S):			MAR	PAT	140:	4066	35									

I

AB Title compds. I [A = (un)substituted aryl, 5 or 6-membered heterocycly! ring, bicyclic heterocycly! B = Ph, pyridy!, Z = 0, S, S0, etc.; R1 = CO2R4, CN, CONR5R6, etc.; R2a, R2b = H, halogen, (un)substituted alkyl, etc., Rx = (un)substituted alkyl, CQa0b-heterocyclyl, CQa0b-bicyclic heterocyclyl, etc.; R4, R5 = H, (un)substituted alkyl, R6 = H, (un)substituted alkyl, heteroaryl, etc.; R8, R9 = H, Cl, F, etc.; Qa, Ob = H, CH3) and their pharmaceutically acceptable derive. were prepared For example, the Suzuki coupling of Et 2'-bromobiphenyl-3-carboxylate and 2-benzyloxy-5-chlorophenylboronic acid, e.g., prepared from 3-ethoxycarbonylphenylboronic acid, followed by hydrolysis afforded compound I [A-R1 = 3-carboxyphenyl; Z = O; R2a = H, R2b = 5-C1; R8, R9 = H] in 39% overall yield. In human prostanoid BPI receptor binding asasys, 90-examples of compds. I exhibited plC50 values ranging from 6.0->9.0

at the EPI receptor and pIC50 values of <6.0 at the EP3 receptor. Of note, no toxicol. effects are indicated/expected (sic) when the compds. I are administered at the assay concentration of 3 nM. Compds. I are claimed useful for the treatment of prostaglandin mediated diseases, e.g., inflammation, pain, etc.

690259-48-4P 690259-49-5P 690259-50-8P

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690259-51-9P 690259-52-0P 690259-53-1P
     690259-54-2P 690259-55-3P 690259-56-4P
     690259-57-5P 690259-58-6P 690259-59-7P
    690259-60-0P 690259-61-1P 690259-62-2P
    690259-63-3P 690259-64-4P 690259-65-5P
    690259-66-6P 690259-67-7P 690259-68-8P
    690259-69-9P 690259-70-2P 690259-71-3P
    690259-72-4P 690259-73-5P 690259-75-7P
    690259-76-8P 690259-77-9P 690259-78-0P
    690259-80-4P 690259-81-5P 690259-82-6P
    690259-84-8P 690259-85-9P 690259-91-7P
    690259-92-8P 690259-93-9P 690259-94-0P
    690259-95-1P 690259-96-2P 690259-97-3P
     690259-98-4P 690259-99-5P 690260-00-5P
    690260-01-6P 690260-02-7P 690260-03-8P
    690260-04-9P 690260-05-0P 690260-06-1P
    690260-07-2P 690260-08-3P 690260-09-4P
    690260-10-7P 690260-11-8P 690260-12-9P
    690260-13-0P 690260-14-1P 690260-15-2P
    690260-16-3P 690260-17-4P 690260-18-5P
    690260-19-6P 690260-20-9P 690260-21-0P
    690260-02-1P 690260-23-2P 690260-24-3P
    690260-25-4P 690260-26-5P 690260-27-6P
    690260-28-7P 690260-29-8P 690260-30-1P
    690260-31-2P 690260-32-3P 690260-33-4P
    690260-34-5P 690260-35-6P 690260-36-7P
     690260-37-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of benzoic acids and related compds. as EP1 receptor
       antagonists for the treatment of prostaglandin mediated diseases.)
RN
    690259-48-4 ZCAPLUS
```

[1.1':2'.1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)-

(9CI) (CA INDEX NAME)

CN

RN 690259-49-5 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3-acetic acid, 5''-chloro-2''-(phenylmethoxy)(9C1) (CA INDEX NAME)

RN 690259-50-8 ZCAPLUS

RN 690259-51-9 ZCAPLUS

RN 690259-52-0 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5-(acetylamino)-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-53-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxopropyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-54-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(2-methyl-1oxopropyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-55-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxobutyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-56-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(benzoylamino)-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-57-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5[(methylsulfonyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-58-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-amino-5''-chloro-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-59-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxobutyl)amino]-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

- RN 690259-60-0 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-chloro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690259-61-1 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690259-62-2 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690259-63-3 ZCAPLUS

[1,1':2',1''-Terphenyl]-3-carboxylic acid, 4-amino-2''-(phenylmethoxy)-CN (9CI) (CA INDEX NAME)

[1,1':2',1''-Terphenyl]-2-carboxylic acid, 5-(acetylamino)-2''-CN (phenylmethoxy) - (9CI) (CA INDEX NAME)

Ph_ CH2_ O

[1,1':2',1''-Terphenyl]-2-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)-CN (9CI) (CA INDEX NAME)

- RN 690259-67-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

- RN 690259-68-8 ZCAPLUS

- RN 690259-69-9 ZCAPLUS
- CN 1H-Tetrazole, 5-[5''-chloro-2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-3-yl]- (9CI) (CA INDEX NAME)

- RN 690259-70-2 ZCAPLUS
- CN [1,1:2',1''-Terphenyl]-2-carboxamide, 5''-chloro-2''-(phenylmethoxy)-N-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 690259-71-3 ZCAPLUS

RN 690259-72-4 ZCAPLUS

CN Benzamide, 4-nitro-N-[[2''-(phenylmethoxy)[1,1':2',1''-terphenyl]-4yl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 690259-73-5 ZCAPLUS

RN 690259-75-7 ZCAPLUS CN [1,1':2',1''-Terphenv1]-3-carbo

N [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4-fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-76-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(2,4-difluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-77-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4chlorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-78-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4-chloro-2fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

RN 690259-80-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-81-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(4-pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-82-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3pyridinylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-84-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3thienylmethoxy)- (9CI) (CA INDEX NAME)



RN 690259-85-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2thienylmethoxy)- (9CI) (CA INDEX NAME)

RN 690259-91-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)-, monomethyl ester (9CI) (CA INDEX NAME)

RN 690259-92-8 ZCAPLUS

RN 690259-93-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-methoxy-2''-(phenylmethoxy)(9CI) (CA INDEX NAME)

RN 690259-94-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-[(1-oxopropyl)amino]-5''-(trifluoromethyl)(9C1) (CA INDEX NAME)

RN 690259-95-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxyl-4-[(2-methyl-1-oxopropyl)amino]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-96-2 ZCAPLUS

CN

RN 690259-97-3 ZCAPLUS

[1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-98-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5[(2-methylpropyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690259-99-5 ZCAPLUS

CN 2-Pyrazinecarboxylic acid, 6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

RN 690260-00-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-

[(1-oxopropyl)amino]-5"-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-01-6 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5-[(1-oxopropy1)amino]-2''-(phenylmethoxy)-5''-(trifluoromethy1)- (9CI) (CA INDEX NAME)

RN 690260-02-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4-fluorophenyl)methoxy]5-[(1-oxopropyl)amino]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-03-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(methoxyacetyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-04-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[(2-thienylacetyl)amino]- (9CI) (CA INDEX NAME)

RN 690260-05-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[[(phenylmethoxy)acetyl]amino]- (9CI) (CA INDEX NAME)

RN 690260-06-1 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5-[[(l-acetyl-4piperidinyl)carbonyl]amino]-5''-chloro-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-07-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5'''-chloro-5[(phenylacetyl)amino]-2'''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-08-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5'''-chloro-5-[[(3,5-dimethyl-4isoxazolyl)carbonyl]amino]-2'''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-09-4 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(3-methyl-1-oxobutyl)amino]-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-10-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(aminoacetyl)amino]-5''chloro-2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-11-8 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-2-carboxylic acid, 4-[(1-oxopropy1)amino]-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-12-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-[(2-methyl-1-oxopropyl)amino]2''-(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-13-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-[(2,4difluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-14-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-bromo-5-cyano-2''(phenylmethoxy)- (9CI) (CA INDEX NAME)

RN 690260-15-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-16-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(aminocarbonyl)-2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CO}_2\text{H} \\ \text{F}_3\text{C} \\ \text{C}_{\text{C}} \\ \text{C}_{\text{H}_2} \\ \end{array}$$

RN 690260-17-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-[((2-hydroxyethyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-18-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5-[((3-pyridinylmethyl)amino]carbonyl]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-19-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-20-9 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-fluorophenyl)methoxy][1,1'biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-21-0 ZCAPLUS
- CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4-difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

- RN 690260-22-1 ZCAPLUS
- CN 4-Pyridinecarboxylic acid, 2-[2'-[(4-fluorophenyl)methoxy]-5'- (trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

RN 690260-23-2 ZCAPLUS

CN 2-Pyrazinecarboxylic acid, 3-amino-6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

RN 690260-24-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''(phenylmethoxy)-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-25-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(4-fluorophenyl)methoxyl-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-26-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4-difluorophenyl)methoxy]-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 690260-27-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-methyl-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

RN 690260-28-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-methyl-5''-(trifluoromethyl)- (9CI) (CA INDEX
NAME)

- RN 690260-29-8 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690260-30-1 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-[(4-fluorophenyl)methoxy]- (9CI) (CA INDEX NAME)

- RN 690260-31-2 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5''-fluoro- (9CI) (CA INDEX NAME)

RN 690260-32-3 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[5-chloro-2-(phenylmethoxy)-3pyridinyl]- (CA INDEX NAME)

RN 690260-33-4 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[6-chloro-3-(phenylmethoxy)-2pyridinyl]- (CA INDEX NAME)

RN 690260-34-5 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-amino-2'-[6-chloro-3-(phenylmethoxy)2-pyridinyl]- (CA INDEX NAME)

RN 690260-35-6 ZCAPLUS

CN 3-Pyridinecarboxylic acid, 5-[2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-(CA INDEX NAME)

- RN 690260-36-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4''-chloro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- RN 690260-37-8 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 6-fluoro-2''-(phenylmethoxy)-(9CI) (CA INDEX NAME)

- IT 690261-75-7
 - RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of benzoic acids and related compds. as EP1 receptor antaconists for the treatment of prostaglandin mediated diseases.)
- RN 690261-75-7 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(2,4-difluorophenyl)methoxyl-5''-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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IT 690260-39-0P 690260-42-5P 690260-45-8P
    690260-47-0P 690260-49-2P 690260-50-5P
    690260-51-6P 690260-52-7P 690260-53-8P
     690260-54-9P 690260-55-0P 690260-57-2P
    690260-60-7P 690260-61-8P 690260-62-9P
    690360-63-0P 690260-64-1P 690260-65-3P
    690260-66-3P 690260-72-1P 690260-73-2P
    690260-74-3P 690260-75-4P 690260-77-6P
    690260-78-7P 690260-79-8P 690260-81-2P
    690260-82-3P 690261-01-9P 690261-06-4P
    690261-07-5P 690261-08-6P 690261-09-7P
     690261-10-0P 690261-12-2P 690261-13-3P
    690261-14-4P 690261-15-5P 690261-16-6P
    690261-17-7P 690261-18-8P 690261-19-9P
    690261-20-2P 690261-21-3P 690261-22-4P
    690361-23-5P 690261-24-6P 690261-25-7P
    690261-26-8P 690261-27-9P 690261-30-4P
    690261-32-6P 690261-33-7P 690261-36-0P
    690261-37-1P 690261-40-6P 690261-41-7P
    690261-42-8P 690261-44-0P 690261-45-1P
    690261-48-4P 690261-49-5P 690261-50-8P
    690261-52-0P 690261-55-3P 690261-56-4P
    690261-57-5P 690261-61-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of benzoic acids and related compds. as EP1 receptor
        antagonists for the treatment of prostaglandin mediated diseases.)
RN
    690260-39-0 ZCAPLUS
    [1,1':2',1''-Terphenvl]-3-carboxvlic acid, 5''-chloro-2''-(phenvlmethoxv)-
CN
     , ethyl ester (9CI) (CA INDEX NAME)
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RN 690260-42-5 ZCAPLUS
CN [1,1':2',1''-Terphenyl]-3-acetic acid, 5''-chloro-2''-(phenylmethoxy)-,
ethyl ester (9CI) (CA INDEX NAME)
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RN 690260-45-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-acetic acid, 5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-47-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-4-acetic acid, 5''-chloro-2''-(phenylmethoxy)-,
ethyl ester (9CI) (CA INDEX NAME)

RN 690260-49-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-amino-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-50-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(acetylamino)-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-51-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxopropyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-52-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(2-methyl-1oxopropyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-53-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(1oxobutyl)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-54-9 ZCAPLUS
- CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5-(benzoylamino)-5''-chloro-2''(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-55-0 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[bis(methylsulfonyl)amino]-5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

- RN 690260-57-2 ZCAPLUS
- CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[(1-oxobutyl)amino]-2''- (phenylmethoxy)-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-60-7 ZCAPLUS

N 690260-61-8 ZCAPLUS

RN 690260-62-9 ZCAPLUS

RN 690260-63-0 ZCAPLUS

RN 690260-64-1 ZCAPLUS

RN 690260-65-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5''-chloro-2''-(phenylmethoxy), ethyl ester (9CI) (CA INDEX NAME)

RN 690260-66-3 ZCAPLUS

RN 690260-72-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4fluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-73-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(2,4-difluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-74-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4chlorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-75-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-[(4-chloro-2-fluorophenyl)methoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-77-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-78-7 ZCAPLUS

CN [1,1:2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(4-pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-79-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3-pyridinylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-81-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(3thienylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690260-82-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(2-thienylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-01-9 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5[((2-methylpropyl)amino]carbonyl]-5''-(trifluoromethyl)-, methyl ester
(SCI) (CA INDEX NAME)

RN 690261-06-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 5-chloro-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-07-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-amino-2''-(phenylmethoxy)-,
methyl ester (9CI) (CA INDEX NAME)

RN 690261-08-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4difluorophenyl)methoxy]-5''-(trifluoromethyl)-, methyl ester (9C1) (CA
INDEX NAME)

RN 690261-09-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-[(1-oxopropyl)amino]-5''-(trifluoromethyl)-,
methyl ester (9C1) (CA INDEX NAMES)

RN 690261-10-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-4-((2-methyl-1-oxopropyl)amino]-5''-(trifluoromethyl)-, methyl ester [9CI) (CA INDEX NAME)

RN 690261-12-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-bromo-5-cyano-2''-(phenylmethoxy)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 690261-13-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-cyano-2''-(phenylmethoxy)-5''(trifluoromethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 690261-14-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-(2-oxo-1-pyrrolidinyl)-2''(phenylmethoxy)-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-15-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3,5-dicarboxylic acid, 2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 690261-16-6 ZCAPLUS

RN 690261-17-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(4-fluorophenyl)methoxy]-5[(1-oxopropyl)amino]-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-18-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5-[(1-oxopropyl)amino]-5''-(trifluoromethyl)-,
methyl ester (9C1) (CA INDEX NAME)

RN 690261-19-9 ZCAPLUS

CN [1,1':2',1''-Terpheny1]-3-carboxylic acid, 5''-chloro-5[(methoxyacety1)amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-20-2 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[(2-thienylacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-21-3 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-2''-(phenylmethoxy)5-[[(phenylmethoxy)acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-22-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5-[[(1-acetyl-4piperidinyl)carbonyl]amino]-5''-chloro-2''-(phenylmethoxy)-, ethyl ester (9C1) (CA INDEX NAME)

RN 690261-23-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[[(3,5-dimethyl-4-isoxazolyl)carbonyl]amino]-2''-(phenylmethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-24-6 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[(3-methyl-1oxobutyl)amino]-2''-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-25-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-chloro-5-[[[[(9H-fluoren-9ylmethoxy)carbonyl]amino]acetyl]amino]-2''-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

- RN 690261-26-8 ZCAPLUS

- RN 690261-27-9 ZCAPLUS
- CN [1,1:2',1''-Terphenyl]-2-carboxylic acid, 4-[(2-methyl-1-oxopropyl)amino]-2''-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN 690261-30-4 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-32-6 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(4-fluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-33-7 ZCAPLUS

CN 2-Pyridinecarboxylic acid, 6-[5'-chloro-2'-[(2,4-difluorophenyl)methoxy][1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-36-0 ZCAPLUS

CN 4-Pyridinecarboxylic acid, 2-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-37-1 ZCAPLUS

CN 2-Pyrazinecarboxylic acid, 3-amino-6-[2'-[(4-fluorophenyl)methoxy]-5'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-40-6 ZCAPLUS

RN 690261-41-7 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(4fluorophenyl)methoxy]-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-42-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-(acetylamino)-2''-[(2,4-difluorophenyl)methoxy]-5''-(trifluoromethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 690261-44-0 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4-methyl-2''-(phenylmethoxy)-,
ethyl ester (9CI) (CA INDEX NAME)

RN 690261-45-1 ZCAPLUS

RN 690261-48-4 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-(phenylmethoxy)-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 690261-49-5 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 5''-fluoro-2''-[(4fluorophenyl)methoxy]-, (4-fluorophenyl)methyl ester (9CI) (CA INDEX NAME)

RN 690261-50-8 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-3-carboxylic acid, 2''-[(2,4difluorophenyl)methoxy]-5''-fluoro-, (2,4-difluorophenyl)methyl ester
(9C1) (CA INDEX NAME)

RN 690261-52-0 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[5-chloro-2-(phenylmethoxy)-3pyridinyl]-, ethyl ester (CA INDEX NAME)

RN 690261-55-3 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-[6-chloro-3-(phenylmethoxy)-2pyridinyl]-, ethyl ester (CA INDEX NAME)

RN 690261-56-4 ZCAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-amino-2'-[6-chloro-3-(phenylmethoxy)-2-pyridinyl]-, methyl ester (CA INDEX NAME)

RN 690261-57-5 ZCAPLUS

CN 3-Pyridinecarboxylic acid, 5-[2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]-, ethyl ester (CA INDEX NAME)

RN 690261-61-1 ZCAPLUS

CN [1,1':2',1''-Terphenyl]-2-carboxylic acid, 4''-chloro-2''-(phenylmethoxy), ethyl ester (9CI) (CA INDEX NAME)



L50 ANSWER 9 OF 13 ZCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:154202 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:187653

TITLE: Preparation of tetracyclic tetrahydroquinoline inhibitors of serine proteases as antithrombotic

agents

Zhou, Jinglan; Robinson, Leslie; Gubernator, Nikolaus; INVENTOR(S):

Saiah, Eddine; Bai, Xu; Gu, Xin Bristol-Myers Squibb Company, USA PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 311 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				TE	APPLICATION NO.									
WO 2003015715 WO 2003015715					WO 2002-US26967									
	AE, AG, CO, CR,	AL, AM, CU, CZ,	AT, A	U, AZ, K, DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
	GM, HR, LS, LT, PL, PT,	LU, LV,	MA, M	MD, MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
RW:	UA, UG, GH, GM,	UZ, VC, KE, LS,	VN, Y MW, M	U, ZA, IZ, SD,	ZM, SL,	ZW SZ,	TZ,	UG,	ZM,	zw,	AM,	AZ,	BY,	
	KG, KZ, FI, FR,	GB, GR,	IE, I	T, LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,			
AU 2002331707			A1 20030303			ML, MR, NE, SN, TD, AU 2002-331707 US 2002-223860					20020820			
			A2 20040609			EP 2002-768687								
R: PRIORITY APP	AT, BE, IE, SI,	LT, LV,			CY,	AL,	TR,	BG,	CZ,	EE,	SK			
OTHER SOURCE(S):			US 2001-313549P P WO 2002-US26967 W MARPAT 138:187653											

179

AB

(shown as I; variables defined below; e.g. 6-(3-chlorophenyl) - 5,6a,7,11btetrahydro-6H-indeno[2,1-c]guinoline-3-carboxamidine), and analogs thereof, and pharmaceutically acceptable salt forms thereof, which are selective inhibitors of serine protease enzymes, especially factor VIIa; pharmaceutical compns. containing the same; and methods of using the same as anticoagulant agents for modulation of the coaquiation cascade. Although the methods of preparation are not claimed, 240 example prepns, are included, Compds, I demonstrated Ki values of ≤50 µM in assays of inhibition of 5 coaqulation factors; values for specific I are not given. For I: X is -NH-, -O-, -S-, -S(O)-, or -S(O)2-; ring A, including the two atoms of Ring B to which it is attached, is a Ph ring; wherein, in addition to RA, ring A is substituted with 0-3 RAA; alternatively, ring A, including the two atoms of Ring B to which it is attached, is a 5-6 membered aromatic system consisting of C atoms and 1 or 2 N atoms, and ring A, in addition to RA, is substituted with 0-3 RAA; alternatively ring A and substituent RA, including the two atoms of Ring B to which ring A is attached, is a 5-6 membered heterocyclic ring; alternatively ring A and substituent RA, including the two atoms of Ring B to which Ring A is attached, is a Ph ring wherein RA is combined with RAA and two C atoms of Ring A to form a cyclic group. RA = F, Cl, Br, OH, OCH3, OCH2CH3, OCHMe2, -OCH2CH2CH3, -OCF3, -CN, -NH2, -NH2NH3, C(:NR1)NR2R3, R-NHC(:NR1)NR2R3, -NR2CH(:NR1), -C(0)NR2R3, -S(0)2NR2aR31, -NR2R3, -CH2NR2R3, -CH2CH2NR2R3, -CHMeNR2R3, -CH2CH2CH2NR2R3, -CH2CHMeNR2R3, -CHEtNR2R3, -CHMeCH2NR2R3, -CMe2NR2R3, -(C1-3alky1)CO2H, -O-(C1-3 alky1)CO2H, -S-(C1-3 alky1)CO2H, and -(C1-3 alky1)CH(NH2)CO2H, -C(0)NHCH2CH2NH(C1-3 alky1), -C(0)NHCH2CH2N(C1-3 alkvl)2, -CH2NCOO(C1-4 alkvl), imidazol-1-vl, substituted 2,5-dihvdro-5oxopyrazol-3-yl, 4,5-dihydroimidazol-2-ylamino, and 1,4,5,6tetrahydropyrimidin-2-ylamino. RB is a 5-10 membered ring system consisting of C atoms and 0, 1 or 2 heteroatoms N, O, and S; wherein said ring system may be unsatd., partially unsatd. or saturated; and RB is substituted with 0-5 substituents = Rb1, Rb2, Rb3, Rb4, and Rb5; alternatively RB is C1-4 alkyl substituted with 5-10 membered ring system consisting of C atoms and 0, 1 or 2 heteroatoms N. O. and S; wherein said ring system may be unsatd., partially unsatd. or saturated; and RB is substituted with 0-5 substituents = Rb1, Rb2, Rb3, Rb4, and Rb5. N is 1, 2, or 3; RC1 = H, halo, -CN, -NO2, OR12, SR12, NR12R13, C(0)H, C(0)R12, C(0)NR12R13, OC(0)NR12R13, NR14C(0)R12, NR14C(S)R12, C(0)OR12, OC(0)R12, OC(0)OR12, CH(:NR14)NR12R13, NHC(:NR14)NR12R13, S(0)R12, S(0)2R12, S(0)NR12R13, S(0)2NR12R13, NR14S(0)R12, NR14S(0)2R12, NR12C(0)R15,

This invention relates generally to tetracyclic tetrahydroguinoline compds.

ΙT

NR12C(5)R15, NR12C(0)OR15, NR12S(0)ZR15, NR12C(0)NRR15, Cl-4 haloalkyl, (Cl-4 haloalkyl)oxy, Cl-10 alkyl substituted with 0-3 RCC, C2-10 alkynyl substituted with 0-3 RCC, C2-10 alkynyl substituted with 0-3 RCC, C1-10 alkoxy substituted with 0-3 RCC, C1-10 alkoxy substituted with 0-3 RCC, C2-10 alkoxyl substituted with 0-3 RCC, aryl substituted with 0-5 RCC, and 5-6 membered heterocyclic ring system containing = 1-4 heteroatoms N, O, and S substituted with 0-3 RCC; RC2 = H, Cl-4 alkyl, OH, CN, and C1-4 alkoxy. Ring D, including the two atoms of Ring C to which it is attached, is a 5-6 membered aromatic system consisting of C atoms and 0, 1 or 2 heteroatoms N, O, and S; and ring D is substituted with 0-4 RD; addnl. details regarding the above variables are given in the claims.

499217-88-9P, 6-(2'-Benzyloxy-5-hydroxy-4-methoxybiphenyl-2-yl)5,6a,7,1lb-tetrahydro-6H-indeno[2,1-c]quinoline-2-carboxamidine
499216-30-3P, 6-(2-Aminomethyl-5,6a,7,1lb-tetrahydro-6H-indeno[2,1-c]quinolin-6-yl)-2'-benzyloxy-4-methoxybiphenyl-3-ol
RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; preparation of tetracyclic tetrahydroquinoline inhibitors of serine proteases as antithrombotic agents)

N 499217-88-8 ZCAPLUS

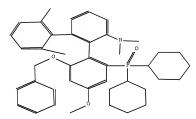
CN 5H-Indeno[2,1-c]quinoline-2-carboximidamide, 6,6a,7,11b-tetrahydro-6-[5-hydroxy-4-methoxy-2'-(phenylmethoxy)[1,1'-biphenyl]-2-yl]- (CA INDEX NAME)

RN 499218-30-3 ZCAPLUS CN [1.1'-Biphenyll-3-ol

[1,1'-Biphenyl]-3-ol, 6-[2-(aminomethyl)-6,6a,7,11b-tetrahydro-5H-indeno[2,1-c]quinolin-6-yl]-4-methoxy-2'-(phenylmethoxy)- (CA INDEX NAME)

L50 ANSWER 10 OF 13 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 10961913 C42 H52 N O3 P Molec. Formula (MF): Molecular Weight (MW): 649.85 Lawson Number (LN): 16731, 16730, 5228, 2817, 289 Compound Type (CTYPE): isocyclic Constitution ID (CONSID): 9165571 Tautomer ID (TAUTID): 10214894 Entry Date (DED): 2008/01/25 Update Date (DUPD): 2008/01/25



Field Availability:

Code	Name	Occurrence
======		
BRN	Beilstein Records	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	5
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Сс	ode	Name	Occurrence
RX		Reaction Documents	1
RX	PRO	Substance is Reaction Product	1

All References:

 Ashburn, Bradley O.; Carter, Rich G.; Zakharov, Lev N., J. Am. Chem. Soc., CODEN: JACSAT, SIR129(29), <2007>, 9109 - 9116; BABS-6702500

L50 ANSWER 11 OF 13 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 10932565 Molec. Formula (MF): C28 H27 N O2 Molecular Weight (MW): 409.53 Lawson Number (LN): 15281, 5228, 289 Compound Type (CTYPE): isocyclic Constitution ID (CONSID): 9141835 10184903 Tautomer ID (TAUTID): Entry Date (DED): 2008/01/25 2008/01/25 Update Date (DUPD):

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
=======		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References: ALLREF

 Ashburn, Bradley O.; Carter, Rich G.; Zakharov, Lev N., J. Am. Chem. Soc., CODEN: JACSAT, SIR129(29), <2007>, 9109 - 9116; BABS-6702500

L50 ANSWER 12 OF 13 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9109439

Chemical Name (CN): 2-<4'-(tert-butyl-dimethyl-

silanyloxymethyl)-6-methoxy-4,2',6'-tris-(4-methoxy-benzyloxy)-biphenyl-2-yl>-4,4-

dimethyl-4,5-dihydro-oxazole

Autonom Name (AUN): 2-<4'-(tert-butyl-dimethyl-

silanyloxymethyl)-6-methoxy-4,2',6'-tris-

(4-methoxy-benzyloxy)-biphenyl-2-yl>-4,4-dimethyl-4,5-dihydro-oxazole

Molec. Formula (MF): C49 H59 N O9 Si

Molecular Weight (MW): 834.09

Lawson Number (LN): 31103, 5917, 3798, 3777, 289

Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7699321 Tautomer ID (TAUTID): 8554879 Entry Date (DED): 2002/07/19 Update Date (DUPD): 2002/07/19

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrenc
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	5
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name C	ccurrence
=======		
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

1. Fuerstner, Alois; Stelzer, Frank; Rumbo, Antonio; Krause, Helga,

Chem.Europ.J., CODEN: CEUJED, 8(8), <2002>, 1856 - 1871; BABS-6340976

L50 ANSWER 13 OF 13 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 9107305

Chemical Name (CN): 2-<4'-(tert-butyl-dimethyl-

silanyloxymethyl)-6-methoxy-2',6'-bis-(4-

methoxy-benzyloxy)-4-methoxymethoxybiphenvl-2-vl>-4,4-dimethyl-4,5-dihydro-

oxazole

Autonom Name (AUN): 2-<4'-(tert-butyl-dimethyl-

silanyloxymethyl)-6-methoxy-2',6'-bis-(4-

methoxy-benzyloxy)-4-methoxymethoxybiphenyl-2-yl>-4,4-dimethyl-4,5-dihydro-

oxazole

Molec. Formula (MF): C43 H55 N O9 Si

Molecular Weight (MW): 757.99 Lawson Number (LN): 31103, 5917, 3798, 3777, 689, 289

Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7697695
Tautomer ID (TAUTID): 8552823

Entry Date (DED): 2002/07/19 Update Date (DUPD): 2002/07/19

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	6
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPR	O Substance is Reaction	Product 1

All References:

 Fuerstner, Alois; Stelzer, Frank; Rumbo, Antonio; Krause, Helga, Chem.Europ.J., CODEN: CEUJED, 8(8), <2002>, 1856 - 1871; BABS-6340976 => => file wpix FILE 'WPIX' ENTERED AT 10:36:08 ON 12 MAY 2008 COPYRIGHT (C) 2008 THOMSON REUTERS

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MOST RECENT THOMSON SCIENTIFIC UPDATE: 200829 < 200829/DW>
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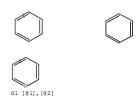
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- => d stat que L53 L1 STR
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L3 $$\operatorname{\mathtt{STR}}$$

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. ${\tt L4}$ ${\tt STR}$

G1



Structure attributes must be viewed using STN Express query preparation. L9 $$\operatorname{\mathtt{STR}}$$



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PROCESSING COMPLETED FOR L53
L54
10 DUP REM L12 L53 (2 DUPLICATES REMOVED)
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ANSWER '10' FROM FILE WPIX

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L54 ANSWER 10 OF 10 WPIX COPYRIGHT 2008 THOMSON REUTERS on STN

ACCESSION NUMBER: 2007-524981 [51] WPIX Full-text DOC. NO. CPI: C2007-193716 [51]

TITLE: New diarylimidazole compounds are cannabinoid receptor

modulators used for treatment or prophylaxis of e.g. obesity, psychiatric disorders, schizophrenia and bipolar disorders, anxiety, depression, cancer and cognitive

disorders

DERWENT CLASS: B03

AHLOVIST M; CHENG L; LUNDOVIST R; SOERENSEN H INVENTOR:

PATENT ASSIGNEE: (ASTR-C) ASTRAZENECA AB; (ASTR-C) ASTRAZENECA UK LTD

COUNTRY COUNT. 115

PATENT INFO ABBR.:

PATENT	NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 200	7031720	A1 2	20070322	(200751)*	EN	55[0]		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION DATE
WO 20070317	720 A1	WO 2006-GB3356 20060912

PRIORITY APPLN. INFO: GB 2005-18817

20050915 AN 2007-524981 [51] WPIX Full-text

AB WO 2007031720 A1 UPAB: 20070809

NOVELTY - Diarylimidazole compounds (I) in the form of their methanesulfonate salts (mesylate salt), hemi-1,5-naphthalenedisulfonate salts, hemi-1,2ethanedisulfonic acid salts, ethylsulfonate salts, nitrate salts,

hydrochloride salts, sulfate salts and hydrogen sulfate salts, are new. DETAILED DESCRIPTION - Diarylimidazole compounds of formula (I) in the

form of their methanesulfonate salts (mesylate salts), hemi-1,5naphthalenedisulfonate salts, hemi-1,2-ethanedisulfonic acid salts,

ethylsulfonate salts and nitrate salts, are new.

R1 = 1-10C alkoxy (optionally substituted by F), phenyl(CH2)pO (optionally substituted by 1-3 Z), R5S(O)20, R5S(O)2NH or (R6)3Si;

p = 1-3;

R5 = 1-10C alkyl (optionally substituted by F), or phenyl or heteroaryl (both optionally substituted by 1-3 Z);

R6 = 1-6C alkyl;

Ra = halo 1-3C alkvl or 1-3C alkoxv;

R2 = 1-3C alkyl, 1-3 alkoxy, OH, NO2, CN or halo;

R2 = 1-3C alkyl, 1-3C alkoxy, OH, NO2, CN or halo;

R3 = X-Y1-NR7R8;

X = CO or SO2;

Y1 = NH, 1-3C alkv1;

R8 = 1-6C alkyl, 3-15C cycloalkyl, (3-15C cycloalkyl)1-3C alkylene (all optionally substituted by 1-3 W1), (-CH2)r(phenyl)s (optionally substituted by 1-3 Z), saturated 5-8 membered heterocyclic group (containing 1 N and optionally O, S or an additional N and optionally substituted by 1-3C alkyl, OH or benzyl), -(CH2)tHet, where the alkylene chain is optionally substituted by 1-3C alkyl; and

R7 = H or R8; or

NR7R8 = saturated or partially unsaturated 5-8 membered heterocyclic group (containing 1 N and optionally one of O, S or an additional N and optionally substituted by 1-3C alkyl, OH, F or benzyl), oxazolyl, isoxazolyl, thiazolyl, isothiazolyl, oxadiazolyl, thiadiazolyl, pyrrolyl, pyrazolyl, imidazolyl, triazolyl, tetrazolyl, thienyl, furyl or oxazolinyl (all optionally substituted by 1-3 Z);

R4 = H, 1-6C alkyl, 1-6C alkoxy, 1-6C alkoxy1-6C alkylene (which contains a maximum of 6 C atoms and all optionally substituted by F or CN);

Z = 1-3C alkyl, 1-3C alkoxy, OH, halo, -CF3, trifluoromethylthio, difluoromethoxy, -OCF3, trifluoromethylsulfonyl, NO2, amino, mono or dil-3c alkylamino, 1-3C alkylsulfonyl, 1-3C alkoxycarbonyl, carboxy, CN, carbamoyl, mono or di-1-3C alkyl carbamovl and acetyl:

W1 = OH, F, 1-3C alkvl, 1-3C alkoxv, NH2, mono or dil-3C alkvlamino or a heterocyclic amine of morpholinyl, pyrrolidinyl, piperidinyl or piperazinyl in which the heterocyclic amine is optionally substituted by 1-3C alkyl or OH;

- m = 0-3;n = 0-3:
- r = 0-4; and
- t = 0-4.

provided that r is 0 otherwise s is 1 or 2; when n is 1 then R2 is not -OCH3 in either the 2-position or the 4- position of the phenyl ring; and R1 is not methylsulfonylamino, -OCH3 or CF30.

ACTIVITY - Anorectic; Neuroleptic; Tranquilizer; Antidepressant; Nootropic; Anabolic; Eating-Disorders-Gen.; Anticonvulsant; Neuroprotective; Antiparkinsonian; Immunomodulator; Cardiovascular-Gen.; Gynecological; Endocrine-Gen.; Antibacterial; Immunosuppressive; Respiratory-Gen.; Gastrointestinal-Gen.; Vasotropic; Antismoking; Hypnotic; Cerebroprotective; Anticoagulant: Analgesic: Antianginal: Antiinfertility: Contraceptive: Antiinflammatory; Hepatotropic; Antiasthmatic; Cytostatic; Antiarthritic.

MECHANISM OF ACTION - Cannabinoid receptor modulator.

In an assay used to determine affinity for central cannaboid receptors as described in Devane et al, Molecular Pharmacology, 1988, 34,605, using membranes prepared from cells stably transfected with the CB 1 gene, results showed that (I) exhibited IC50 values of less than 200 nm.

USE - Used for the treatment or prophylaxis of obesity, psychiatric disorders such as psychotic disorders, schizophrenia and bipolar disorders, anxiety, anxio-depressive disorders, depression, cognitive disorders, memory disorders, obsessive-compulsive disorders, anorexia, bulimia, attention disorders, epilepsy and related conditions, neurological disorders, Parkinson's disease, Huntington's chorea, Alzheimer's disease, immune, cardiovascular, reproductive and endocrine disorders, septic shock, diseases related to the respiratory and gastrointestinal systems and extended abuse, addiction and/or relapse indications (claimed). (I) are useful e.g. to prevent weight gain, for modulation of appetite and/or satiety, eating disorders, to treat Tourette's syndrome, multiple sclerosis, Raynaud's syndrome, nicotine withdrawal, sleep disorder, cranial trauma, sleep apnea, stroke, cerebral apoplexy, ischemia, cerebral thrombosis, metabolic syndrome, syndrome X, reproductive and endocrine disorders, infertility, contraceptive, qastrointestinal systems, cholelithiasis, asthma, chronic obstructive pulmonary disease, cancer, Prader-Willi syndrome, arthritis and orthopedic disorders.

ADVANTAGE - (I) are in crystalline form. (I) are more efficacious, less toxic, longer acting, more potent and more easily absorbed. (I) has a broader range of activity, a better pharmacokinetic profile (e.g. higher oral bioavailability and/or lower clearance) and pharmacological, physical or chemical properties. (I) are administered less frequently. (I) exhibits improved ease of handling. (I) may be produced in forms which may have improved chemical and/or solid state stability (e.g. due to lower hygroscopicity). (I) are stable over prolonged periods. (I) are crystallised in good yields, in a high purity and at a low cost. (I) has potency, selectivity profile, half-life in plasma, blood brain permeability, plasma protein binding (higher free fraction of drug) or solubility.

CN.S THIOPHENE-2-SULFONIC ACID 4-[2-(2,4-DICHLORO-PHENYL)-5-METHYL-4-(PIPERIDIN-1-YLCARBANOYL)-IMIDAZOL-1-YL]-PHENYL ESTER HYDROCHLORIDE
SDCN RAOWSI

AN.S DCR-1502117

- CN.S 5-Chloro-thiophene-2-sulfonic acid 4-[2-(2,4-dichloro-pheny1)-5-methy1-4-(piperidin-1-ylcarbamoy1)-imidazol-1-yl]-phenyl ester hydrochloride SDCN RAQW9P
- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT * AN.S DCR-1502378
- CN.S Pyridine-3-sulfonic acid 4-[2-(2,4-dichloro-phenyl)-5-methyl-4-(piperidin-1-ylcarbamoyl)-imidazol-1-yl]-phenyl ester hydrochloride SDCN RAGWGR

L13

1.14

L15

=> d his full

(FILE 'HOME' ENTERED AT 10:01:19 ON 12 MAY 2008)

FILE 'REGISTRY' ENTERED AT 10:01:23 ON 12 MAY 2008

L1 STRUCTURE UPLOADED L2 0 SEA SSS SAM L1

L3 STRUCTURE UPLOADED
L4 STRUCTURE UPLOADED

L5 SCREEN 1841 L6 SCREEN 1946

L6 SCREEN 1946 L7 5110201 SEA ARR=ON

L7 5110201 SEA ABB=ON PLU=ON 46.150.18/RID AND NRS>3

L8 0 SEA SUB=L7 SSS SAM (L1 AND L3 AND L4) AND (L5 AND L6)
L9 STRUCTURE UPLOADED
L10 1 SEA SUB=L7 SSS SAM (L1 AND L3 AND L4 AND L9) AND (L5 AND L6)

D SCA
L11 239 SEA SUB=L7 SSS FUL (L1 AND L3 AND L4 AND L9) AND (L5 AND L6)
SAVE TEMP VALO36ST1349/A L11

FILE 'ZCAPLUS' ENTERED AT 10:13:16 ON 12 MAY 2008

L12 9 SEA ABB=ON PLU=ON L11 D BIB HITSTR L12 9

E US2006-533036 /APPS

2 SEA ABB=ON PLU=ON US2006-533036 /AP D SCA

1 SEA ABB=ON PLU=ON US2005-533036 /AP D SCA D AU

1 SEA ABB=ON PLU=ON L12 AND L14 D SCA

SEL RN SEL HIT RN

FILE 'REGISTRY' ENTERED AT 10:17:27 ON 12 MAY 2008

L16 295 SEA ABB=ON PLU=ON (100-39-0/BI OR 100398-25-2/BI OR 1007-16-5 /BI OR 107-82-4/BI OR 108-24-7/BI OR 121-43-7/BI OR 124-63-0/BI OR 13659-23-9/BI OR 136808-72-5/BI OR 137628-16-1/BI OR 14067-99-3/BI OR 141-43-5/BI OR 141-75-3/BI OR 150255-96-2/BI OR 176548-70-2/BI OR 179897-94-0/BI OR 188057-26-3/BI OR 188815-32-9/BI OR 190661-29-1/BI OR 200956-32-7/BI OR 202409-82 -3/BI OR 204841-19-0/BI OR 207115-22-8/BI OR 20986-40-7/BI OR 21190-88-5/BT OR 21739-93-5/BT OR 21856-53-1/BT OR 22921-67-1/B I OR 23915-07-3/BI OR 244205-40-1/BI OR 26628-22-8/BI OR 353743-43-8/BI OR 363-24-6/BI OR 3637-61-4/BI OR 3731-52-0/BI OR 380430-56-8/BI OR 3808-91-1/BI OR 402-45-9/BI OR 41288-96-4/ BI OR 4214-79-3/BI OR 4334-87-6/BI OR 459-46-1/BI OR 4635-59-0/ BI OR 5419-55-6/BI OR 557-21-1/BI OR 583-53-9/BI OR 60-12-8/BI OR 612832-83-4/BI OR 612833-40-6/BI OR 612833-41-7/BI OR 612833-60-0/BI OR 612833-61-1/BI OR 612833-62-2/BI OR 612833-63 -3/BI OR 612833-64-4/BI OR 612833-65-5/BI OR 612833-66-6/BI OR 612833-67-7/BI OR 612833-68-8/BI OR 612833-69-9/BI OR 612833-70 -2/BI OR 612833-71-3/BI OR 612833-72-4/BI OR 612833-73-5/BI OR 6307-83-1/BI OR 690259-48-4/BI OR 690259-49-5/BI OR 690259-50-8 /BI OR 690259-51-9/BI OR 690259-52-0/BI OR 690259-53-1/BI OR 690259-54-2/BI OR 690259-55-3/BI OR 690259-56-4/BI OR 690259-57 -5/BI OR 690259-58-6/BI OR 690259-59-7/BI OR 690259-60-0/BI OR 690259-61-1/BI OR 690259-62-2/BI OR 690259-63-3/BI OR 690259-64 -4/BI OR 690259-65-5/BI OR 690259-66-6/BI OR 690259-67-7/BI OR

L17

L18 L19 690259-68-8/BI OR 690259-69-9/BI OR 690259-70-2/BI OR 690259-71
-3/BI OR 690259-72-4/BI OR 690259-73-5/BI OR 690259-74-6/BI OR
690259-75-7/BI OR 690259-76-8/BI OR 690259-77-9/BI OR 690259-78
-0/BI OR 690259-79-1/BI OR 690259-80-4/BI OR 690259-81-5/BI OR
690259-82-6/BI OR 690259-83-7/BI OR 690259-84-8/BI OR 690259-85
-9/BI OR

151 SEA ABB=ON PLU=ON (690259-48-4/BI OR 690259-49-5/BI OR 690259-50-8/BI OR 690259-51-9/BI OR 690259-52-0/BI OR 690259-53 -1/BI OR 690259-54-2/BI OR 690259-55-3/BI OR 690259-56-4/BI OR 690259-57-5/BI OR 690259-58-6/BI OR 690259-59-7/BI OR 690259-60 -0/BI OR 690259-61-1/BI OR 690259-62-2/BI OR 690259-63-3/BI OR 690259-64-4/BI OR 690259-65-5/BI OR 690259-66-6/BI OR 690259-67 -7/BI OR 690259-68-8/BI OR 690259-69-9/BI OR 690259-70-2/BI OR 690259-71-3/BI OR 690259-72-4/BI OR 690259-73-5/BI OR 690259-75 -7/BI OR 690259-76-8/BI OR 690259-77-9/BI OR 690259-78-0/BI OR 690259-80-4/BI OR 690259-81-5/BI OR 690259-82-6/BI OR 690259-84 -8/BI OR 690259-85-9/BI OR 690259-91-7/BI OR 690259-92-8/BI OR 690259-93-9/BI OR 690259-94-0/BI OR 690259-95-1/BI OR 690259-96 -2/BI OR 690259-97-3/BI OR 690259-98-4/BI OR 690259-99-5/BI OR 690260-00-5/BI OR 690260-01-6/BI OR 690260-02-7/BI OR 690260-03 -8/BI OR 690260-04-9/BI OR 690260-05-0/BI OR 690260-06-1/BI OR 690260-07-2/BI OR 690260-08-3/BI OR 690260-09-4/BI OR 690260-10 -7/BI OR 690260-11-8/BI OR 690260-12-9/BI OR 690260-13-0/BI OR 690260-14-1/BI OR 690260-15-2/BI OR 690260-16-3/BI OR 690260-17 -4/BI OR 690260-18-5/BI OR 690260-19-6/BI OR 690260-20-9/BI OR 690260-21-0/BI OR 690260-22-1/BI OR 690260-23-2/BI OR 690260-24 -3/BI OR 690260-25-4/BI OR 690260-26-5/BI OR 690260-27-6/BI OR 690260-28-7/BI OR 690260-29-8/BI OR 690260-30-1/BI OR 690260-31 -2/BI OR 690260-32-3/BI OR 690260-33-4/BI OR 690260-34-5/BI OR 690260-35-6/BI OR 690260-36-7/BI OR 690260-37-8/BI OR 690260-39 -0/BI OR 690260-42-5/BI OR 690260-45-8/BI OR 690260-47-0/BI OR 690260-49-2/BI OR 690260-50-5/BI OR 690260-51-6/BI OR 690260-52 -7/BI OR 690260-53-8/BI OR 690260-54-9/BI OR 690260-55-0/BI OR 690260-57-2/BI OR 690260-60-7/BI OR 690260-61-8/BI OR 690260-62 -9/BI OR 690260-63-0/BI OR 690260-64-1/BI OR 690

144 SEA ABB=ON PLU=ON L16 NOT L17 5 SEA ABB=ON PLU=ON L18 AND NRS>3

D SCA

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1.20
           151 SEA ABB=ON PLU=ON L11 AND L16
     FILE 'ZCAPLUS' ENTERED AT 10:19:49 ON 12 MAY 2008
L21
            3 SEA ABB=ON PLU=ON L20
L22
            19 SEA ABB=ON PLU=ON BIT R?/AU
L23
            89 SEA ABB=ON PLU=ON GIBLIN G?/AU
L24
          2354 SEA ABB=ON PLU=ON HALL A?/AU
L25
           319 SEA ABB=ON PLU=ON HURST D?/AU
L26
            13 SEA ABB=ON PLU=ON KILFORD I?/AU
L27
          1179 SEA ABB=ON PLU=ON MILLER N?/AU
L28
            13 SEA ABB=ON PLU=ON SCOCCITTI T?/AU
L29
             8 SEA ABB=ON PLU=ON L22 AND (L23 OR L24 OR L25 OR L26 OR L27
               OR L28)
1.30
            34 SEA ABB=ON PLU=ON L23 AND (L24 OR L25 OR L26 OR L27 OR L28)
L31
            33 SEA ABB=ON PLU=ON L24 AND (L25 OR L26 OR L27 OR L28)
            18 SEA ABB=ON PLU=ON L25 AND (L26 OR L27 OR L28)
L32
L33
            5 SEA ABB=ON PLU=ON L26 AND (L27 OR L28)
L34
            2 SEA ABB=ON PLU=ON L27 AND L28
L35
            7 SEA ABB=ON PLU=ON L29 AND (L30 OR L31 OR L32 OR L33 OR L34)
L36
           19 SEA ABB=ON PLU=ON L30 AND (L31 OR L32 OR L33 OR L34)
L37
           17 SEA ABB=ON PLU=ON L31 AND (L32 OR L33 OR L34)
            4 SEA ABB=ON PLU=ON L32 AND (L33 OR L34)
L38
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10/533036
1.39
            2 SEA ABB=ON PLU=ON L33 AND L34
L40
            21 SEA ABB=ON PLU=ON (L35 OR L36 OR L37 OR L38 OR L39)
             3 SEA ABB=ON PLU=ON L21 AND (L22 OR L23 OR L24 OR L25 OR L26
L41
               OR L27 OR L28)
             3 SEA ABB=ON PLU=ON L12 AND (L22 OR L23 OR L24 OR L25 OR L26
L42
               OR L27 OR L28)
    FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:24:53 ON 12 MAY 2008
L43
            27 SEA ABB=ON PLU=ON L40
    FILE 'BEILSTEIN' ENTERED AT 10:25:28 ON 12 MAY 2008
             0 SEA SSS SAM (L1 AND L3 AND L4 AND L9)
L44
            13 SEA SSS FUL (L1 AND L3 AND L4 AND L9)
L45
1.46
            9 SEA ABB=ON PLU=ON L45 AND BABSAN/FA
L47
             4 SEA ABB=ON PLU=ON L45 NOT L46
               SEL BABSAN L46
    FILE 'BABS' ENTERED AT 10:27:21 ON 12 MAY 2008
L48
             4 SEA ABB=ON PLU=ON (6644860/BABSAN OR 6702500/BABSAN OR
               6340976/BABSAN OR 6562995/BABSAN)
    FILE 'REGISTRY' ENTERED AT 10:28:00 ON 12 MAY 2008
    FILE 'ZCAPLUS' ENTERED AT 10:28:09 ON 12 MAY 2008
               D STAT OUE L40
               D STAT QUE L43
    FILE 'REGISTRY' ENTERED AT 10:28:41 ON 12 MAY 2008
    FILE 'ZCAPLUS' ENTERED AT 10:28:45 ON 12 MAY 2008
               D STAT OUE L40
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FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:29:00 ON 12 MAY 2008 D STAT QUE L43

FILE 'ZCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 10:29:20 ON 12 MAY 2008

L49 22 DUP REM L40 L43 (26 DUPLICATES REMOVED)
ANSWERS '1-21' FROM FILE ZCAPLUS
ANSWER '22' FROM FILE BIOSIS

D IBIB ABS L49 1-21 D IALL L49 22

FILE 'REGISTRY' ENTERED AT 10:30:20 ON 12 MAY 2008

FILE 'ZCAPLUS' ENTERED AT 10:30:27 ON 12 MAY 2008 D STAT QUE L21 D IBIB ABS HITSTR L21 1-3

FILE 'REGISTRY' ENTERED AT 10:31:02 ON 12 MAY 2008

FILE 'ZCAPLUS' ENTERED AT 10:31:07 ON 12 MAY 2008 D STAT QUE L12

FILE 'BABS' ENTERED AT 10:31:22 ON 12 MAY 2008 D STAT QUE L48

FILE 'BEILSTEIN' ENTERED AT 10:31:38 ON 12 MAY 2008 D STAT QUE L47

FILE 'ZCAPLUS, BABS, BEILSTEIN' ENTERED AT 10:31:59 ON 12 MAY 2008

13 DUP REM L12 L48 L47 (4 DUPLICATES REMOVED)
ANSWERS '1-9' FROM FILE ZCAPLUS

ANSWERS '10-13' FROM FILE BEILSTEIN

D IBIB ABS HITSTR L50 1-9 D IDE ALLREF L50 10-13

FILE 'WPIX' ENTERED AT 10:35:03 ON 12 MAY 2008

L51 8 SEA SSS SAM L1 AND L3 AND L4 AND L9

L52 109 SEA SSS FUL L1 AND L3 AND L4 AND L9

L53 3 SEA ABB=ON PLU=ON L52/DCR

FILE 'WPIX' ENTERED AT 10:36:08 ON 12 MAY 2008 D STAT QUE L53

FILE 'ZCAPLUS, WPIX' ENTERED AT 10:36:30 ON 12 MAY 2008 L54 10 DUP REM L12 L53 (2 DUPLICATES REMOVED)

ANSWERS '1-9' FROM FILE ZCAPLUS
ANSWER '10' FROM FILE WPIX
D IBIB ABS HITSTR L54 10

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAY 2008 HIGHEST RN 1020256-26-1 DICTIONARY FILE UPDATES: 11 MAY 2008 HIGHEST RN 1020256-26-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE ZCAPLUS

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FILE COVERS 1907 - 12 May 2008 VOL 148 ISS 20 FILE LAST UPDATED: 11 May 2008 (20080511/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE MEDITNE

FILE LAST UPDATED: 10 May 2008 (20080510/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

FILE EMBASE

FILE COVERS 1974 TO 12 May 2008 (20080512/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 12 May 2008 (20080512/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED:

MAY 2008 <20080504/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE:

DERMENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<</p>

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomsonreuters/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0: http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.p

- >>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<
- >>> Updated PDF files in the following links: http://www.stn-international.de/stndatabases/details/ico 0803.zip http://www.stn-international.de/stndatabases/details/epc_0803.zip Supplement of all changed ECLA items: http://www.stn-international.de/stndatabases/details/ecla_0803s.zip <<
- >>> Please note that the COPYRIGHT notification has changed <<<

FILE BEILSTEIN FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008. FILE CONTAINS 10.322,808 SUBSTANCES

- >>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<
- >>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

- * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
- * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
- * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE
- * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
- * FOR PRICE INFORMATION SEE HELP COST -
- >>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

FILE BARS

FILE LAST UPDATED: 17 MAR 2008 <20080317/UP>

FILE COVERS 1980 TO DATE.

Uploading L1.str

chain nodes :

13 14 15 16 17 18 19 20 21 23 30 33 34 38 40 41 42 43 44 45 46 47 48 49 54 55

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 chain bonds :

1-38 2-11 12-40 14-15 16-17 18-20 19-20 20-21 30-38 40-54 41-42 41-43 44-45 44-47 46-48 46-49 54-55

ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-38 2-11 7-8 7-12 8-9 9-10 10-11 11-12 12-40 14-15 16-17 18-20 19-20 20-21 30-38 40-54 41-42 41-43 44-45 44-47 46-48 46-49 54-55

normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6

G1:[*1],[*2],[*3],[*4],[*5]

G2:C,N

G3:[*6],[*7]

G4:0.S

G5:[*8],[*9],[*10]

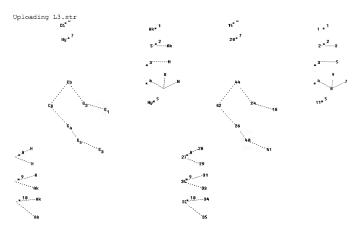
Connectivity:

21:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

```
19:CLASS 20:CLASS 21:CLASS 23:Atom 34:Atom 38:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 46:CLASS 46:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 54:CLASS 55:CLASS 69:CLASS 69:CLASS 64:CLASS 64:CL
```



```
chain nodes:
1 2 3 4 5 6 7 8 9 11 18 19 20 24 26 27 28 29 30 31 32 33 34 34 34 40 41 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44 42 44
```

G1:[*1],[*2],[*3],[*4],[*5]

G3:[*6],[*7]

G4:0,S

G5:[*8],[*9],[*10]

Connectivity:

9:1 E exact RC ring/chain 42:4 X maximum RC ring/chain 44:4 X maximum RC ring/chain

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:Atom 18:CLASS 19:Atom 20:Atom 24:CLASS 26:CLASS 27:CLASS 28:CLASS

29:CLASS 30:CLASS 31:CLASS

32:CLASS 33:CLASS 34:CLASS 35:CLASS 40:CLASS 41:CLASS 42:Atom 44:Atom

Generic attributes :

19:

Saturation 42:

: Unsaturated

Saturation : Unsaturated Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Saturation

: Unsaturated Number of Carbon Atoms : less than 7

Type of Ring System : Monocyclic

Element Count :

Node 42: Limited C, C5-6 N, NO-1

S. S0 0,00

P,P0

Node 44: Limited C, C6

Uploading L4.str







23



chain nodes : 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

ring bonds :

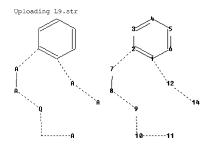
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1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 normalized bonds: 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16 16-17 17-18 isolated fring systems:
```

G1:[*1],[*2]

containing 1 : 7 : 13 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 23:CLASS



```
9 10 ring nodes: 1 2 3 4 5 6 7 8 11 12 14 chain bonds: 1-12 2-7 8-9 9-10 10-11 ring bonds: 1-2 1-6 2-3 3-4 4-5 5-6 7-8 12-14 exact/norm bonds: 1-12 2-7 8-9 9-10 10-11 12-14 normalized bonds: 1-2 1-6 2-3 3-4 4-5 5-6 7-8 isolated ring systems: containing 1:
```

Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS 11:Atom 12:Atom 14:Atom

=>